

The Prevalence of *Iso*closo Deltahedra in Low-Energy Hypoelectronic Metalladiboranes with a Single Metal Vertex: Manganese and Rhenium Derivatives

Alexandru Lupan¹ and R. Bruce King*²

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

²*Department of Chemistry, University of Georgia, Athens, Georgia, 30602*

Supporting Information

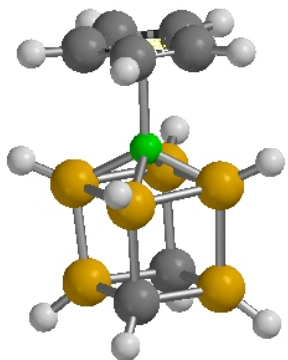
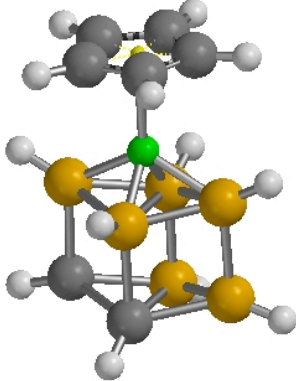
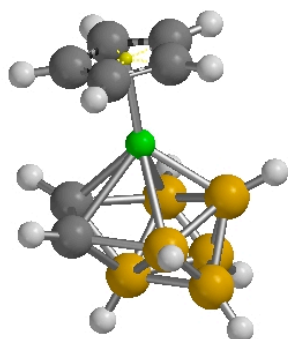
- Details of all of the CpMC₂B_{*n*-3}H_{*n*-2} structures (M = Mn, Re; *n* = 9, 10, 11, 12)
- Complete Gaussian09 reference (reference 35)

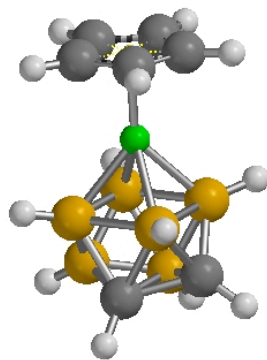
Gaussian 09, Revision A.02,

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.

9-vertex $\text{CpMnC}_2\text{B}_6\text{H}_8$

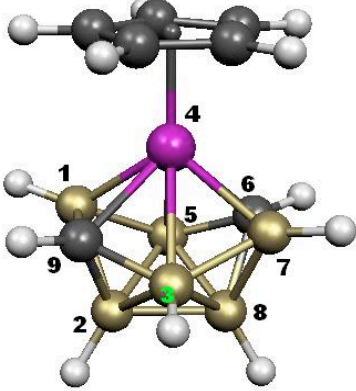
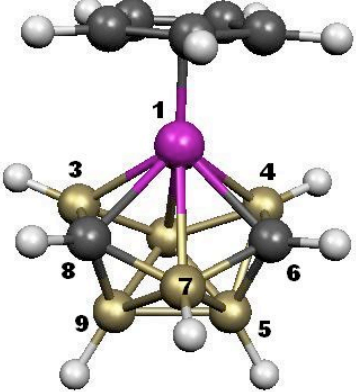
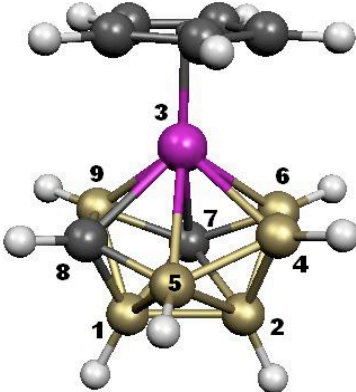
Table 1. Initial structures (one example from each family) 166 structures in total

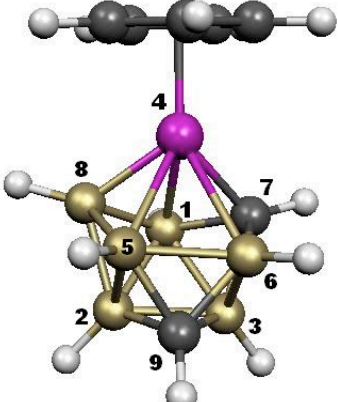
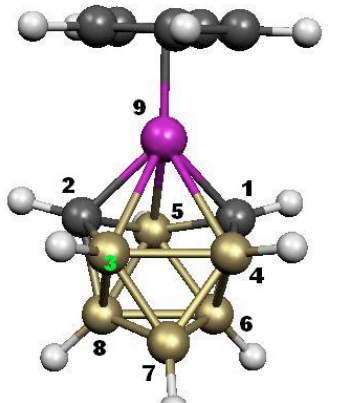
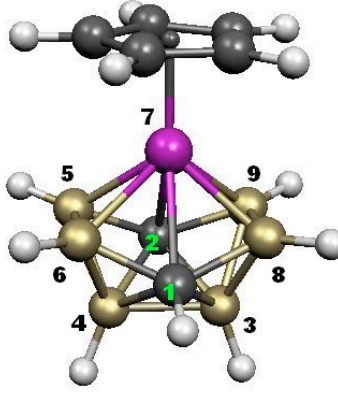
Initial structures
 <p>1. Capped cube 43 structures</p>
 <p>2. Pressed capped cube 29 structures</p>
 <p>3. Tl_9^{9-}-like structure 70 structures</p>

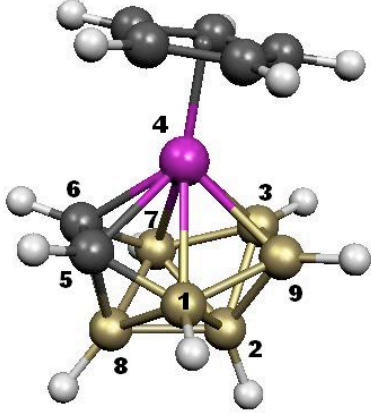
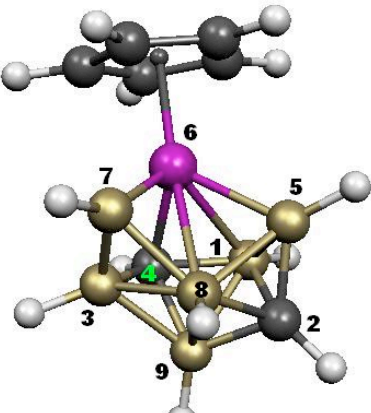
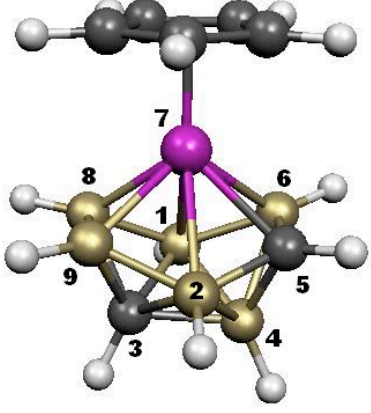


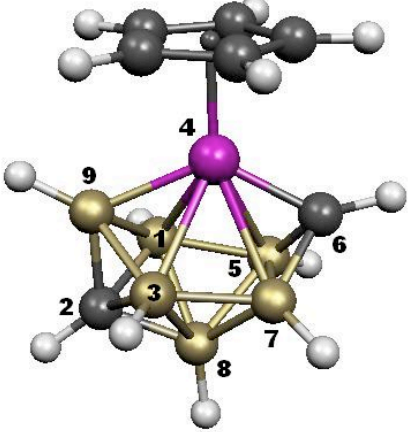
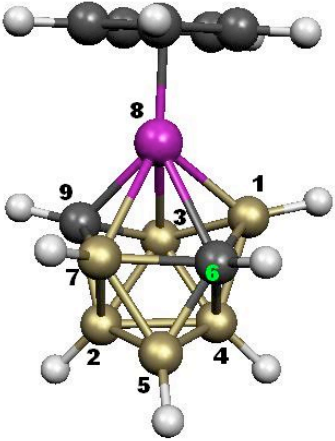
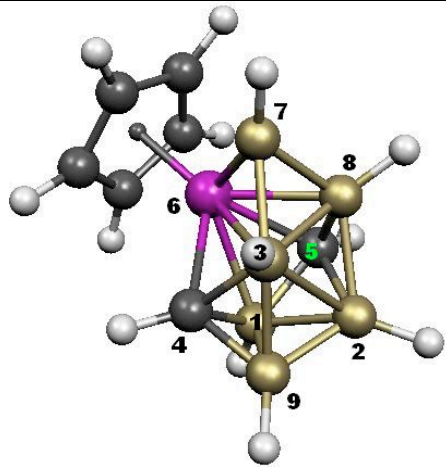
4. Tricapped trigonal prism 24 structures

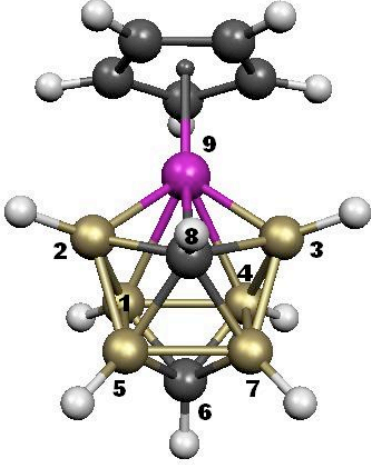
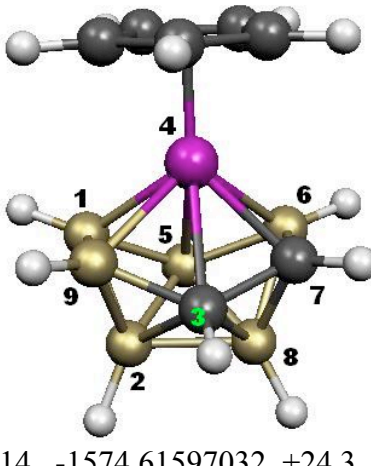
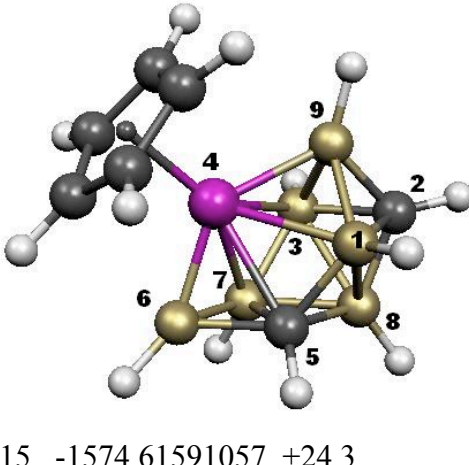
Table 2. Distance table for the best structures

 <p>1. -1574.65469642 C2 0.0 kcal/mole</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.817090</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.705267</td><td>1.851193</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Mn</td><td>2.036163</td><td>2.822550</td><td>2.280148</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.737277</td><td>1.866896</td><td>2.761266</td><td>2.276168</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.857559</td><td>2.759612</td><td>2.593816</td><td>2.029357</td><td>1.583684</td></tr> <tr><td>7 B</td><td>3.360718</td><td>2.933327</td><td>1.736643</td><td>2.037173</td><td>2.704778</td></tr> <tr><td>8 B</td><td>2.935454</td><td>1.794730</td><td>1.869069</td><td>2.822940</td><td>1.851259</td></tr> <tr><td>9 C</td><td>1.554424</td><td>1.640256</td><td>1.583468</td><td>2.032642</td><td>2.593379</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.554512</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.639588</td><td>1.816797</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.127215</td><td>2.856576</td><td>2.761410</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.817090	0.000000				3 B	2.705267	1.851193	0.000000			4 Mn	2.036163	2.822550	2.280148	0.000000		5 B	1.737277	1.866896	2.761266	2.276168	0.000000	6 C	2.857559	2.759612	2.593816	2.029357	1.583684	7 B	3.360718	2.933327	1.736643	2.037173	2.704778	8 B	2.935454	1.794730	1.869069	2.822940	1.851259	9 C	1.554424	1.640256	1.583468	2.032642	2.593379		6	7	8	9		6 C	0.000000					7 B	1.554512	0.000000				8 B	1.639588	1.816797	0.000000			9 C	3.127215	2.856576	2.761410	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.817090	0.000000																																																																																									
3 B	2.705267	1.851193	0.000000																																																																																								
4 Mn	2.036163	2.822550	2.280148	0.000000																																																																																							
5 B	1.737277	1.866896	2.761266	2.276168	0.000000																																																																																						
6 C	2.857559	2.759612	2.593816	2.029357	1.583684																																																																																						
7 B	3.360718	2.933327	1.736643	2.037173	2.704778																																																																																						
8 B	2.935454	1.794730	1.869069	2.822940	1.851259																																																																																						
9 C	1.554424	1.640256	1.583468	2.032642	2.593379																																																																																						
	6	7	8	9																																																																																							
6 C	0.000000																																																																																										
7 B	1.554512	0.000000																																																																																									
8 B	1.639588	1.816797	0.000000																																																																																								
9 C	3.127215	2.856576	2.761410	0.000000																																																																																							
 <p>2. -1574.65140139 Cs +2.1</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 Mn</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.366009</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.087112</td><td>1.711203</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.087053</td><td>1.711243</td><td>2.933000</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.835573</td><td>1.821391</td><td>2.912385</td><td>1.778644</td><td>0.000000</td></tr> <tr><td>6 C</td><td>1.992783</td><td>2.585957</td><td>3.232260</td><td>1.557862</td><td>1.657602</td></tr> <tr><td>7 B</td><td>2.244917</td><td>2.758129</td><td>2.713081</td><td>2.713102</td><td>1.880308</td></tr> <tr><td>8 C</td><td>1.992847</td><td>2.585932</td><td>1.557862</td><td>3.232263</td><td>2.776020</td></tr> <tr><td>9 B</td><td>2.835541</td><td>1.821341</td><td>1.778593</td><td>2.912354</td><td>1.813300</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.602963</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.734600</td><td>1.602931</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.775989</td><td>1.880260</td><td>1.657544</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 Mn	0.000000					2 B	2.366009	0.000000				3 B	2.087112	1.711203	0.000000			4 B	2.087053	1.711243	2.933000	0.000000		5 B	2.835573	1.821391	2.912385	1.778644	0.000000	6 C	1.992783	2.585957	3.232260	1.557862	1.657602	7 B	2.244917	2.758129	2.713081	2.713102	1.880308	8 C	1.992847	2.585932	1.557862	3.232263	2.776020	9 B	2.835541	1.821341	1.778593	2.912354	1.813300		6	7	8	9		6 C	0.000000					7 B	1.602963	0.000000				8 C	2.734600	1.602931	0.000000			9 B	2.775989	1.880260	1.657544	0.000000	
	1	2	3	4	5																																																																																						
1 Mn	0.000000																																																																																										
2 B	2.366009	0.000000																																																																																									
3 B	2.087112	1.711203	0.000000																																																																																								
4 B	2.087053	1.711243	2.933000	0.000000																																																																																							
5 B	2.835573	1.821391	2.912385	1.778644	0.000000																																																																																						
6 C	1.992783	2.585957	3.232260	1.557862	1.657602																																																																																						
7 B	2.244917	2.758129	2.713081	2.713102	1.880308																																																																																						
8 C	1.992847	2.585932	1.557862	3.232263	2.776020																																																																																						
9 B	2.835541	1.821341	1.778593	2.912354	1.813300																																																																																						
	6	7	8	9																																																																																							
6 C	0.000000																																																																																										
7 B	1.602963	0.000000																																																																																									
8 C	2.734600	1.602931	0.000000																																																																																								
9 B	2.775989	1.880260	1.657544	0.000000																																																																																							
 <p>3. -1574.64188329 +8.0</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.799727</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Mn</td><td>2.819820</td><td>2.797371</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.916790</td><td>1.767996</td><td>2.044834</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.829233</td><td>1.867518</td><td>2.249981</td><td>1.742540</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.874291</td><td>1.753503</td><td>2.072481</td><td>1.669996</td><td>2.739748</td></tr> <tr><td>7 C</td><td>1.741725</td><td>1.769251</td><td>2.212400</td><td>2.622988</td><td>2.613009</td></tr> <tr><td>8 C</td><td>1.642375</td><td>2.775433</td><td>2.031623</td><td>2.887776</td><td>1.590700</td></tr> <tr><td>9 B</td><td>1.809038</td><td>2.909238</td><td>2.049965</td><td>3.356828</td><td>2.682848</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 C</td><td>1.621644</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>3.246447</td><td>2.453541</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.885004</td><td>1.621623</td><td>1.548472</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.799727	0.000000				3 Mn	2.819820	2.797371	0.000000			4 B	2.916790	1.767996	2.044834	0.000000		5 B	1.829233	1.867518	2.249981	1.742540	0.000000	6 B	2.874291	1.753503	2.072481	1.669996	2.739748	7 C	1.741725	1.769251	2.212400	2.622988	2.613009	8 C	1.642375	2.775433	2.031623	2.887776	1.590700	9 B	1.809038	2.909238	2.049965	3.356828	2.682848		6	7	8	9		6 B	0.000000					7 C	1.621644	0.000000				8 C	3.246447	2.453541	0.000000			9 B	2.885004	1.621623	1.548472	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.799727	0.000000																																																																																									
3 Mn	2.819820	2.797371	0.000000																																																																																								
4 B	2.916790	1.767996	2.044834	0.000000																																																																																							
5 B	1.829233	1.867518	2.249981	1.742540	0.000000																																																																																						
6 B	2.874291	1.753503	2.072481	1.669996	2.739748																																																																																						
7 C	1.741725	1.769251	2.212400	2.622988	2.613009																																																																																						
8 C	1.642375	2.775433	2.031623	2.887776	1.590700																																																																																						
9 B	1.809038	2.909238	2.049965	3.356828	2.682848																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 C	1.621644	0.000000																																																																																									
8 C	3.246447	2.453541	0.000000																																																																																								
9 B	2.885004	1.621623	1.548472	0.000000																																																																																							

 <p>4. -1574.63883303 +10.0</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.850882</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.862982</td><td>1.843695</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Mn</td><td>2.163357</td><td>3.048587</td><td>3.070644</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.682993</td><td>1.899759</td><td>2.664511</td><td>2.237375</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.663489</td><td>2.645187</td><td>1.847936</td><td>2.284168</td><td>1.918785</td></tr> <tr><td>7 C</td><td>1.635926</td><td>2.729667</td><td>1.654710</td><td>1.892614</td><td>2.762370</td></tr> <tr><td>8 B</td><td>1.767103</td><td>1.795576</td><td>2.936662</td><td>1.924077</td><td>1.780551</td></tr> <tr><td>9 C</td><td>2.706304</td><td>1.608458</td><td>1.615670</td><td>3.148244</td><td>1.605478</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 C</td><td>1.636197</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.956418</td><td>2.744456</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.598095</td><td>2.569663</td><td>2.743537</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.850882	0.000000				3 B	1.862982	1.843695	0.000000			4 Mn	2.163357	3.048587	3.070644	0.000000		5 B	2.682993	1.899759	2.664511	2.237375	0.000000	6 B	2.663489	2.645187	1.847936	2.284168	1.918785	7 C	1.635926	2.729667	1.654710	1.892614	2.762370	8 B	1.767103	1.795576	2.936662	1.924077	1.780551	9 C	2.706304	1.608458	1.615670	3.148244	1.605478		6	7	8	9		6 B	0.000000					7 C	1.636197	0.000000				8 B	2.956418	2.744456	0.000000			9 C	1.598095	2.569663	2.743537	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.850882	0.000000																																																																																									
3 B	1.862982	1.843695	0.000000																																																																																								
4 Mn	2.163357	3.048587	3.070644	0.000000																																																																																							
5 B	2.682993	1.899759	2.664511	2.237375	0.000000																																																																																						
6 B	2.663489	2.645187	1.847936	2.284168	1.918785																																																																																						
7 C	1.635926	2.729667	1.654710	1.892614	2.762370																																																																																						
8 B	1.767103	1.795576	2.936662	1.924077	1.780551																																																																																						
9 C	2.706304	1.608458	1.615670	3.148244	1.605478																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 C	1.636197	0.000000																																																																																									
8 B	2.956418	2.744456	0.000000																																																																																								
9 C	1.598095	2.569663	2.743537	0.000000																																																																																							
 <p>5. -1574.63512069 Cs +12.3</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 C</td><td>2.586000</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.768614</td><td>1.628502</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.628438</td><td>2.768488</td><td>1.938500</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.622716</td><td>1.622635</td><td>2.657841</td><td>2.657804</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.640405</td><td>2.744678</td><td>2.657437</td><td>1.852644</td><td>1.907149</td></tr> <tr><td>7 B</td><td>2.716068</td><td>2.716143</td><td>1.707284</td><td>1.707304</td><td>2.903728</td></tr> <tr><td>8 B</td><td>2.744625</td><td>1.640658</td><td>1.852662</td><td>2.657364</td><td>1.907149</td></tr> <tr><td>9 Mn</td><td>1.905467</td><td>1.905684</td><td>2.276085</td><td>2.275740</td><td>2.135572</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>1.724924</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.872300</td><td>1.724843</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Mn</td><td>3.088284</td><td>3.335503</td><td>3.088511</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 C	2.586000	0.000000				3 B	2.768614	1.628502	0.000000			4 B	1.628438	2.768488	1.938500	0.000000		5 B	1.622716	1.622635	2.657841	2.657804	0.000000	6 B	1.640405	2.744678	2.657437	1.852644	1.907149	7 B	2.716068	2.716143	1.707284	1.707304	2.903728	8 B	2.744625	1.640658	1.852662	2.657364	1.907149	9 Mn	1.905467	1.905684	2.276085	2.275740	2.135572		6	7	8	9		6 B	0.000000					7 B	1.724924	0.000000				8 B	1.872300	1.724843	0.000000			9 Mn	3.088284	3.335503	3.088511	0.000000	
	1	2	3	4	5																																																																																						
1 C	0.000000																																																																																										
2 C	2.586000	0.000000																																																																																									
3 B	2.768614	1.628502	0.000000																																																																																								
4 B	1.628438	2.768488	1.938500	0.000000																																																																																							
5 B	1.622716	1.622635	2.657841	2.657804	0.000000																																																																																						
6 B	1.640405	2.744678	2.657437	1.852644	1.907149																																																																																						
7 B	2.716068	2.716143	1.707284	1.707304	2.903728																																																																																						
8 B	2.744625	1.640658	1.852662	2.657364	1.907149																																																																																						
9 Mn	1.905467	1.905684	2.276085	2.275740	2.135572																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 B	1.724924	0.000000																																																																																									
8 B	1.872300	1.724843	0.000000																																																																																								
9 Mn	3.088284	3.335503	3.088511	0.000000																																																																																							
 <p>6. -1574.62954536 C2v-like +15.78</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 C</td><td>2.468204</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.743438</td><td>1.743116</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.742292</td><td>1.742029</td><td>1.823683</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.602751</td><td>1.634752</td><td>2.897710</td><td>1.750879</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.634194</td><td>2.602595</td><td>2.897322</td><td>1.750468</td><td>1.662102</td></tr> <tr><td>7 Mn</td><td>2.193451</td><td>2.191655</td><td>2.792568</td><td>2.790591</td><td>2.062075</td></tr> <tr><td>8 B</td><td>1.633477</td><td>2.601513</td><td>1.749919</td><td>2.894724</td><td>3.359147</td></tr> <tr><td>9 B</td><td>2.601783</td><td>1.633564</td><td>1.750227</td><td>2.894895</td><td>2.919441</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 Mn</td><td>2.063685</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.919243</td><td>2.064569</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.359080</td><td>2.063025</td><td>1.661202</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 C	2.468204	0.000000				3 B	1.743438	1.743116	0.000000			4 B	1.742292	1.742029	1.823683	0.000000		5 B	2.602751	1.634752	2.897710	1.750879	0.000000	6 B	1.634194	2.602595	2.897322	1.750468	1.662102	7 Mn	2.193451	2.191655	2.792568	2.790591	2.062075	8 B	1.633477	2.601513	1.749919	2.894724	3.359147	9 B	2.601783	1.633564	1.750227	2.894895	2.919441		6	7	8	9		6 B	0.000000					7 Mn	2.063685	0.000000				8 B	2.919243	2.064569	0.000000			9 B	3.359080	2.063025	1.661202	0.000000	
	1	2	3	4	5																																																																																						
1 C	0.000000																																																																																										
2 C	2.468204	0.000000																																																																																									
3 B	1.743438	1.743116	0.000000																																																																																								
4 B	1.742292	1.742029	1.823683	0.000000																																																																																							
5 B	2.602751	1.634752	2.897710	1.750879	0.000000																																																																																						
6 B	1.634194	2.602595	2.897322	1.750468	1.662102																																																																																						
7 Mn	2.193451	2.191655	2.792568	2.790591	2.062075																																																																																						
8 B	1.633477	2.601513	1.749919	2.894724	3.359147																																																																																						
9 B	2.601783	1.633564	1.750227	2.894895	2.919441																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 Mn	2.063685	0.000000																																																																																									
8 B	2.919243	2.064569	0.000000																																																																																								
9 B	3.359080	2.063025	1.661202	0.000000																																																																																							

 <p>7. -1574.62754352 Cs +17.0</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.874275</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.755446</td><td>1.768521</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Mn</td><td>2.277390</td><td>2.797977</td><td>2.061356</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>1.575772</td><td>2.781168</td><td>3.255308</td><td>2.016722</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.546474</td><td>2.781197</td><td>2.855870</td><td>2.016619</td><td>1.458900</td></tr> <tr><td>7 B</td><td>2.742900</td><td>1.874420</td><td>1.733127</td><td>2.277375</td><td>2.546538</td></tr> <tr><td>8 B</td><td>1.837700</td><td>1.801705</td><td>2.927316</td><td>2.859677</td><td>1.701063</td></tr> <tr><td>9 B</td><td>1.733242</td><td>1.768657</td><td>1.672800</td><td>2.061007</td><td>2.855830</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.575783</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.701126</td><td>1.837788</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.255091</td><td>2.755363</td><td>2.927375</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.874275	0.000000				3 B	2.755446	1.768521	0.000000			4 Mn	2.277390	2.797977	2.061356	0.000000		5 C	1.575772	2.781168	3.255308	2.016722	0.000000	6 C	2.546474	2.781197	2.855870	2.016619	1.458900	7 B	2.742900	1.874420	1.733127	2.277375	2.546538	8 B	1.837700	1.801705	2.927316	2.859677	1.701063	9 B	1.733242	1.768657	1.672800	2.061007	2.855830		6	7	8	9		6 C	0.000000					7 B	1.575783	0.000000				8 B	1.701126	1.837788	0.000000			9 B	3.255091	2.755363	2.927375	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.874275	0.000000																																																																																									
3 B	2.755446	1.768521	0.000000																																																																																								
4 Mn	2.277390	2.797977	2.061356	0.000000																																																																																							
5 C	1.575772	2.781168	3.255308	2.016722	0.000000																																																																																						
6 C	2.546474	2.781197	2.855870	2.016619	1.458900																																																																																						
7 B	2.742900	1.874420	1.733127	2.277375	2.546538																																																																																						
8 B	1.837700	1.801705	2.927316	2.859677	1.701063																																																																																						
9 B	1.733242	1.768657	1.672800	2.061007	2.855830																																																																																						
	6	7	8	9																																																																																							
6 C	0.000000																																																																																										
7 B	1.575783	0.000000																																																																																									
8 B	1.701126	1.837788	0.000000																																																																																								
9 B	3.255091	2.755363	2.927375	0.000000																																																																																							
 <p>8. -1574.62405144 +19.2</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 C</td><td>1.697358</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.696335</td><td>2.805594</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.581360</td><td>2.577596</td><td>1.563318</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.817883</td><td>1.535708</td><td>3.056742</td><td>2.789348</td><td>0.000000</td></tr> <tr><td>6 Mn</td><td>2.240775</td><td>2.892065</td><td>2.154181</td><td>2.014815</td><td>2.016575</td></tr> <tr><td>7 B</td><td>3.458825</td><td>3.286429</td><td>1.749911</td><td>2.850253</td><td>2.854746</td></tr> <tr><td>8 B</td><td>2.569680</td><td>1.662065</td><td>1.865998</td><td>2.572637</td><td>1.899186</td></tr> <tr><td>9 B</td><td>1.868970</td><td>1.590589</td><td>1.842602</td><td>1.676787</td><td>2.674768</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>6 Mn</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.850980</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.323223</td><td>1.805668</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.951393</td><td>3.124546</td><td>1.915223</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.697358	0.000000				3 B	2.696335	2.805594	0.000000			4 C	1.581360	2.577596	1.563318	0.000000		5 B	1.817883	1.535708	3.056742	2.789348	0.000000	6 Mn	2.240775	2.892065	2.154181	2.014815	2.016575	7 B	3.458825	3.286429	1.749911	2.850253	2.854746	8 B	2.569680	1.662065	1.865998	2.572637	1.899186	9 B	1.868970	1.590589	1.842602	1.676787	2.674768		6	7	8	9		6 Mn	0.000000					7 B	1.850980	0.000000				8 B	2.323223	1.805668	0.000000			9 B	2.951393	3.124546	1.915223	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 C	1.697358	0.000000																																																																																									
3 B	2.696335	2.805594	0.000000																																																																																								
4 C	1.581360	2.577596	1.563318	0.000000																																																																																							
5 B	1.817883	1.535708	3.056742	2.789348	0.000000																																																																																						
6 Mn	2.240775	2.892065	2.154181	2.014815	2.016575																																																																																						
7 B	3.458825	3.286429	1.749911	2.850253	2.854746																																																																																						
8 B	2.569680	1.662065	1.865998	2.572637	1.899186																																																																																						
9 B	1.868970	1.590589	1.842602	1.676787	2.674768																																																																																						
	6	7	8	9																																																																																							
6 Mn	0.000000																																																																																										
7 B	1.850980	0.000000																																																																																									
8 B	2.323223	1.805668	0.000000																																																																																								
9 B	2.951393	3.124546	1.915223	0.000000																																																																																							
 <p>9. -1574.62325636 +19.7</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>2.752937</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>1.750504</td><td>1.797745</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.797884</td><td>1.860849</td><td>1.723564</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>2.572520</td><td>1.574451</td><td>2.648673</td><td>1.651613</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.706195</td><td>2.683253</td><td>2.796635</td><td>1.784787</td><td>1.541470</td></tr> <tr><td>7 Mn</td><td>2.329551</td><td>2.243305</td><td>2.657385</td><td>2.831219</td><td>2.053037</td></tr> <tr><td>8 B</td><td>1.702615</td><td>2.736208</td><td>1.683042</td><td>2.879299</td><td>3.252080</td></tr> <tr><td>9 B</td><td>2.747682</td><td>1.709073</td><td>1.705276</td><td>2.909655</td><td>2.860183</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 Mn</td><td>2.099810</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.940980</td><td>2.058130</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.374914</td><td>2.030724</td><td>1.674282</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.752937	0.000000				3 C	1.750504	1.797745	0.000000			4 B	1.797884	1.860849	1.723564	0.000000		5 C	2.572520	1.574451	2.648673	1.651613	0.000000	6 B	1.706195	2.683253	2.796635	1.784787	1.541470	7 Mn	2.329551	2.243305	2.657385	2.831219	2.053037	8 B	1.702615	2.736208	1.683042	2.879299	3.252080	9 B	2.747682	1.709073	1.705276	2.909655	2.860183		6	7	8	9		6 B	0.000000					7 Mn	2.099810	0.000000				8 B	2.940980	2.058130	0.000000			9 B	3.374914	2.030724	1.674282	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	2.752937	0.000000																																																																																									
3 C	1.750504	1.797745	0.000000																																																																																								
4 B	1.797884	1.860849	1.723564	0.000000																																																																																							
5 C	2.572520	1.574451	2.648673	1.651613	0.000000																																																																																						
6 B	1.706195	2.683253	2.796635	1.784787	1.541470																																																																																						
7 Mn	2.329551	2.243305	2.657385	2.831219	2.053037																																																																																						
8 B	1.702615	2.736208	1.683042	2.879299	3.252080																																																																																						
9 B	2.747682	1.709073	1.705276	2.909655	2.860183																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 Mn	2.099810	0.000000																																																																																									
8 B	2.940980	2.058130	0.000000																																																																																								
9 B	3.374914	2.030724	1.674282	0.000000																																																																																							

 <p>10. -1574.62042106 Cs +21.5</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 C</td> <td>1.656982</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 B</td> <td>2.482100</td> <td>1.657058</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 Mn</td> <td>2.258870</td> <td>2.932634</td> <td>2.258530</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 B</td> <td>1.783823</td> <td>2.788081</td> <td>2.787476</td> <td>2.269877</td> <td>0.000000</td> </tr> <tr> <td>6 C</td> <td>2.882917</td> <td>3.644217</td> <td>2.882884</td> <td>1.813274</td> <td>1.559966</td> </tr> <tr> <td>7 B</td> <td>2.787574</td> <td>2.788204</td> <td>1.783884</td> <td>2.269686</td> <td>1.848500</td> </tr> <tr> <td>8 B</td> <td>1.893067</td> <td>1.572286</td> <td>1.893034</td> <td>2.970934</td> <td>1.809642</td> </tr> <tr> <td>9 B</td> <td>1.781746</td> <td>1.561262</td> <td>1.781734</td> <td>2.005262</td> <td>3.042179</td> </tr> <tr> <td></td> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> </tr> <tr> <td>6 C</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>7 B</td> <td>1.559930</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 B</td> <td>2.800350</td> <td>1.809691</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>9 B</td> <td>3.426356</td> <td>3.042263</td> <td>2.655735</td> <td>0.000000</td> <td></td> </tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.656982	0.000000				3 B	2.482100	1.657058	0.000000			4 Mn	2.258870	2.932634	2.258530	0.000000		5 B	1.783823	2.788081	2.787476	2.269877	0.000000	6 C	2.882917	3.644217	2.882884	1.813274	1.559966	7 B	2.787574	2.788204	1.783884	2.269686	1.848500	8 B	1.893067	1.572286	1.893034	2.970934	1.809642	9 B	1.781746	1.561262	1.781734	2.005262	3.042179			6	7	8	9	6 C	0.000000					7 B	1.559930	0.000000				8 B	2.800350	1.809691	0.000000			9 B	3.426356	3.042263	2.655735	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 C	1.656982	0.000000																																																																																									
3 B	2.482100	1.657058	0.000000																																																																																								
4 Mn	2.258870	2.932634	2.258530	0.000000																																																																																							
5 B	1.783823	2.788081	2.787476	2.269877	0.000000																																																																																						
6 C	2.882917	3.644217	2.882884	1.813274	1.559966																																																																																						
7 B	2.787574	2.788204	1.783884	2.269686	1.848500																																																																																						
8 B	1.893067	1.572286	1.893034	2.970934	1.809642																																																																																						
9 B	1.781746	1.561262	1.781734	2.005262	3.042179																																																																																						
		6	7	8	9																																																																																						
6 C	0.000000																																																																																										
7 B	1.559930	0.000000																																																																																									
8 B	2.800350	1.809691	0.000000																																																																																								
9 B	3.426356	3.042263	2.655735	0.000000																																																																																							
 <p>11. -1574.61947993 +22.1</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>2.913536</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 B</td> <td>1.754790</td> <td>1.908131</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 B</td> <td>1.762562</td> <td>1.837613</td> <td>1.829252</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 B</td> <td>2.836245</td> <td>1.704080</td> <td>2.883246</td> <td>1.725560</td> <td>0.000000</td> </tr> <tr> <td>6 C</td> <td>1.667635</td> <td>2.516011</td> <td>2.559111</td> <td>1.792343</td> <td>1.611591</td> </tr> <tr> <td>7 B</td> <td>2.825793</td> <td>1.863492</td> <td>2.638813</td> <td>2.616760</td> <td>1.718159</td> </tr> <tr> <td>8 Mn</td> <td>1.938580</td> <td>3.084030</td> <td>2.184208</td> <td>3.064966</td> <td>3.317373</td> </tr> <tr> <td>9 C</td> <td>2.700499</td> <td>1.661716</td> <td>1.625695</td> <td>2.700785</td> <td>2.730264</td> </tr> <tr> <td></td> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> </tr> <tr> <td>6 C</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>7 B</td> <td>1.769853</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 Mn</td> <td>2.214962</td> <td>2.186353</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>9 C</td> <td>2.647467</td> <td>1.641158</td> <td>1.881963</td> <td>0.000000</td> <td></td> </tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.913536	0.000000				3 B	1.754790	1.908131	0.000000			4 B	1.762562	1.837613	1.829252	0.000000		5 B	2.836245	1.704080	2.883246	1.725560	0.000000	6 C	1.667635	2.516011	2.559111	1.792343	1.611591	7 B	2.825793	1.863492	2.638813	2.616760	1.718159	8 Mn	1.938580	3.084030	2.184208	3.064966	3.317373	9 C	2.700499	1.661716	1.625695	2.700785	2.730264			6	7	8	9	6 C	0.000000					7 B	1.769853	0.000000				8 Mn	2.214962	2.186353	0.000000			9 C	2.647467	1.641158	1.881963	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	2.913536	0.000000																																																																																									
3 B	1.754790	1.908131	0.000000																																																																																								
4 B	1.762562	1.837613	1.829252	0.000000																																																																																							
5 B	2.836245	1.704080	2.883246	1.725560	0.000000																																																																																						
6 C	1.667635	2.516011	2.559111	1.792343	1.611591																																																																																						
7 B	2.825793	1.863492	2.638813	2.616760	1.718159																																																																																						
8 Mn	1.938580	3.084030	2.184208	3.064966	3.317373																																																																																						
9 C	2.700499	1.661716	1.625695	2.700785	2.730264																																																																																						
		6	7	8	9																																																																																						
6 C	0.000000																																																																																										
7 B	1.769853	0.000000																																																																																									
8 Mn	2.214962	2.186353	0.000000																																																																																								
9 C	2.647467	1.641158	1.881963	0.000000																																																																																							
 <p>12. -1574.61947506 +22.1</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr> <td>1 B</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>2 B</td> <td>1.887751</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 B</td> <td>2.536776</td> <td>2.022736</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 C</td> <td>1.676838</td> <td>2.513093</td> <td>1.687507</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 C</td> <td>1.585013</td> <td>1.693430</td> <td>2.565013</td> <td>2.636499</td> <td>0.000000</td> </tr> <tr> <td>6 Mn</td> <td>2.251225</td> <td>2.998745</td> <td>2.218178</td> <td>1.985311</td> <td>2.032648</td> </tr> <tr> <td>7 B</td> <td>3.495306</td> <td>3.199749</td> <td>1.807988</td> <td>2.856576</td> <td>2.861334</td> </tr> <tr> <td>8 B</td> <td>2.674618</td> <td>1.860691</td> <td>1.870287</td> <td>2.883273</td> <td>1.547090</td> </tr> <tr> <td>9 B</td> <td>1.823561</td> <td>1.671470</td> <td>1.824274</td> <td>1.532775</td> <td>2.730049</td> </tr> <tr> <td></td> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> </tr> <tr> <td>6 Mn</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>7 B</td> <td>1.857195</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 B</td> <td>2.138746</td> <td>1.744196</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>9 B</td> <td>3.098490</td> <td>3.523051</td> <td>2.941760</td> <td>0.000000</td> <td></td> </tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.887751	0.000000				3 B	2.536776	2.022736	0.000000			4 C	1.676838	2.513093	1.687507	0.000000		5 C	1.585013	1.693430	2.565013	2.636499	0.000000	6 Mn	2.251225	2.998745	2.218178	1.985311	2.032648	7 B	3.495306	3.199749	1.807988	2.856576	2.861334	8 B	2.674618	1.860691	1.870287	2.883273	1.547090	9 B	1.823561	1.671470	1.824274	1.532775	2.730049			6	7	8	9	6 Mn	0.000000					7 B	1.857195	0.000000				8 B	2.138746	1.744196	0.000000			9 B	3.098490	3.523051	2.941760	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.887751	0.000000																																																																																									
3 B	2.536776	2.022736	0.000000																																																																																								
4 C	1.676838	2.513093	1.687507	0.000000																																																																																							
5 C	1.585013	1.693430	2.565013	2.636499	0.000000																																																																																						
6 Mn	2.251225	2.998745	2.218178	1.985311	2.032648																																																																																						
7 B	3.495306	3.199749	1.807988	2.856576	2.861334																																																																																						
8 B	2.674618	1.860691	1.870287	2.883273	1.547090																																																																																						
9 B	1.823561	1.671470	1.824274	1.532775	2.730049																																																																																						
		6	7	8	9																																																																																						
6 Mn	0.000000																																																																																										
7 B	1.857195	0.000000																																																																																									
8 B	2.138746	1.744196	0.000000																																																																																								
9 B	3.098490	3.523051	2.941760	0.000000																																																																																							

 <p>13. -1574.61903538 Cs +22.4</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.777070</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.925948</td><td>2.811400</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.921500</td><td>2.925583</td><td>1.777082</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.867870</td><td>1.776657</td><td>2.876912</td><td>2.643713</td><td>0.000000</td></tr> <tr><td>6 C</td><td>1.603895</td><td>2.734898</td><td>2.734780</td><td>1.603986</td><td>1.605443</td></tr> <tr><td>7 B</td><td>2.643673</td><td>2.876934</td><td>1.776687</td><td>1.868266</td><td>1.821200</td></tr> <tr><td>8 C</td><td>2.556296</td><td>1.670414</td><td>1.670454</td><td>2.556254</td><td>1.739522</td></tr> <tr><td>9 Mn</td><td>2.262696</td><td>1.917049</td><td>1.916860</td><td>2.262034</td><td>3.048873</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th></th> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.605273</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.569430</td><td>1.739592</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Mn</td><td>3.151163</td><td>3.048817</td><td>2.131483</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.777070	0.000000				3 B	2.925948	2.811400	0.000000			4 B	1.921500	2.925583	1.777082	0.000000		5 B	1.867870	1.776657	2.876912	2.643713	0.000000	6 C	1.603895	2.734898	2.734780	1.603986	1.605443	7 B	2.643673	2.876934	1.776687	1.868266	1.821200	8 C	2.556296	1.670414	1.670454	2.556254	1.739522	9 Mn	2.262696	1.917049	1.916860	2.262034	3.048873		6	7	8	9		6 C	0.000000					7 B	1.605273	0.000000				8 C	2.569430	1.739592	0.000000			9 Mn	3.151163	3.048817	2.131483	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.777070	0.000000																																																																																									
3 B	2.925948	2.811400	0.000000																																																																																								
4 B	1.921500	2.925583	1.777082	0.000000																																																																																							
5 B	1.867870	1.776657	2.876912	2.643713	0.000000																																																																																						
6 C	1.603895	2.734898	2.734780	1.603986	1.605443																																																																																						
7 B	2.643673	2.876934	1.776687	1.868266	1.821200																																																																																						
8 C	2.556296	1.670414	1.670454	2.556254	1.739522																																																																																						
9 Mn	2.262696	1.917049	1.916860	2.262034	3.048873																																																																																						
	6	7	8	9																																																																																							
6 C	0.000000																																																																																										
7 B	1.605273	0.000000																																																																																									
8 C	2.569430	1.739592	0.000000																																																																																								
9 Mn	3.151163	3.048817	2.131483	0.000000																																																																																							
 <p>14. -1574.61597032 +24.3</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.744119</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.614190</td><td>1.786711</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Mn</td><td>2.087552</td><td>2.806916</td><td>2.164798</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.726457</td><td>1.826195</td><td>2.608338</td><td>2.336039</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.959192</td><td>2.918263</td><td>2.581972</td><td>2.084535</td><td>1.703805</td></tr> <tr><td>7 C</td><td>3.239459</td><td>2.770394</td><td>1.520539</td><td>1.997631</td><td>2.568476</td></tr> <tr><td>8 B</td><td>2.910702</td><td>1.821185</td><td>1.780010</td><td>2.838680</td><td>1.801843</td></tr> <tr><td>9 B</td><td>1.668589</td><td>1.769313</td><td>1.635181</td><td>2.048059</td><td>2.742555</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 C</td><td>1.552312</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.781017</td><td>1.674761</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.365130</td><td>2.812855</td><td>2.915552</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.744119	0.000000				3 C	2.614190	1.786711	0.000000			4 Mn	2.087552	2.806916	2.164798	0.000000		5 B	1.726457	1.826195	2.608338	2.336039	0.000000	6 B	2.959192	2.918263	2.581972	2.084535	1.703805	7 C	3.239459	2.770394	1.520539	1.997631	2.568476	8 B	2.910702	1.821185	1.780010	2.838680	1.801843	9 B	1.668589	1.769313	1.635181	2.048059	2.742555		6	7	8	9		6 B	0.000000					7 C	1.552312	0.000000				8 B	1.781017	1.674761	0.000000			9 B	3.365130	2.812855	2.915552	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.744119	0.000000																																																																																									
3 C	2.614190	1.786711	0.000000																																																																																								
4 Mn	2.087552	2.806916	2.164798	0.000000																																																																																							
5 B	1.726457	1.826195	2.608338	2.336039	0.000000																																																																																						
6 B	2.959192	2.918263	2.581972	2.084535	1.703805																																																																																						
7 C	3.239459	2.770394	1.520539	1.997631	2.568476																																																																																						
8 B	2.910702	1.821185	1.780010	2.838680	1.801843																																																																																						
9 B	1.668589	1.769313	1.635181	2.048059	2.742555																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 C	1.552312	0.000000																																																																																									
8 B	1.781017	1.674761	0.000000																																																																																								
9 B	3.365130	2.812855	2.915552	0.000000																																																																																							
 <p>15. -1574.61591057 +24.3</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 C</td><td>1.688618</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.526397</td><td>1.707345</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Mn</td><td>2.200338</td><td>2.931842</td><td>2.270396</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>1.646200</td><td>2.608151</td><td>2.616337</td><td>2.119042</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.941033</td><td>3.792078</td><td>3.054603</td><td>1.867549</td><td>1.634458</td></tr> <tr><td>7 B</td><td>2.714298</td><td>2.731861</td><td>1.722698</td><td>2.188245</td><td>1.692491</td></tr> <tr><td>8 B</td><td>1.957496</td><td>1.564979</td><td>1.906156</td><td>2.977529</td><td>1.711142</td></tr> <tr><td>9 B</td><td>1.785425</td><td>1.545790</td><td>1.781542</td><td>2.021517</td><td>2.861432</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>1.714982</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.970228</td><td>1.782306</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.551183</td><td>2.948885</td><td>2.646593</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.688618	0.000000				3 B	2.526397	1.707345	0.000000			4 Mn	2.200338	2.931842	2.270396	0.000000		5 C	1.646200	2.608151	2.616337	2.119042	0.000000	6 B	2.941033	3.792078	3.054603	1.867549	1.634458	7 B	2.714298	2.731861	1.722698	2.188245	1.692491	8 B	1.957496	1.564979	1.906156	2.977529	1.711142	9 B	1.785425	1.545790	1.781542	2.021517	2.861432		6	7	8	9		6 B	0.000000					7 B	1.714982	0.000000				8 B	2.970228	1.782306	0.000000			9 B	3.551183	2.948885	2.646593	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 C	1.688618	0.000000																																																																																									
3 B	2.526397	1.707345	0.000000																																																																																								
4 Mn	2.200338	2.931842	2.270396	0.000000																																																																																							
5 C	1.646200	2.608151	2.616337	2.119042	0.000000																																																																																						
6 B	2.941033	3.792078	3.054603	1.867549	1.634458																																																																																						
7 B	2.714298	2.731861	1.722698	2.188245	1.692491																																																																																						
8 B	1.957496	1.564979	1.906156	2.977529	1.711142																																																																																						
9 B	1.785425	1.545790	1.781542	2.021517	2.861432																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 B	1.714982	0.000000																																																																																									
8 B	2.970228	1.782306	0.000000																																																																																								
9 B	3.551183	2.948885	2.646593	0.000000																																																																																							

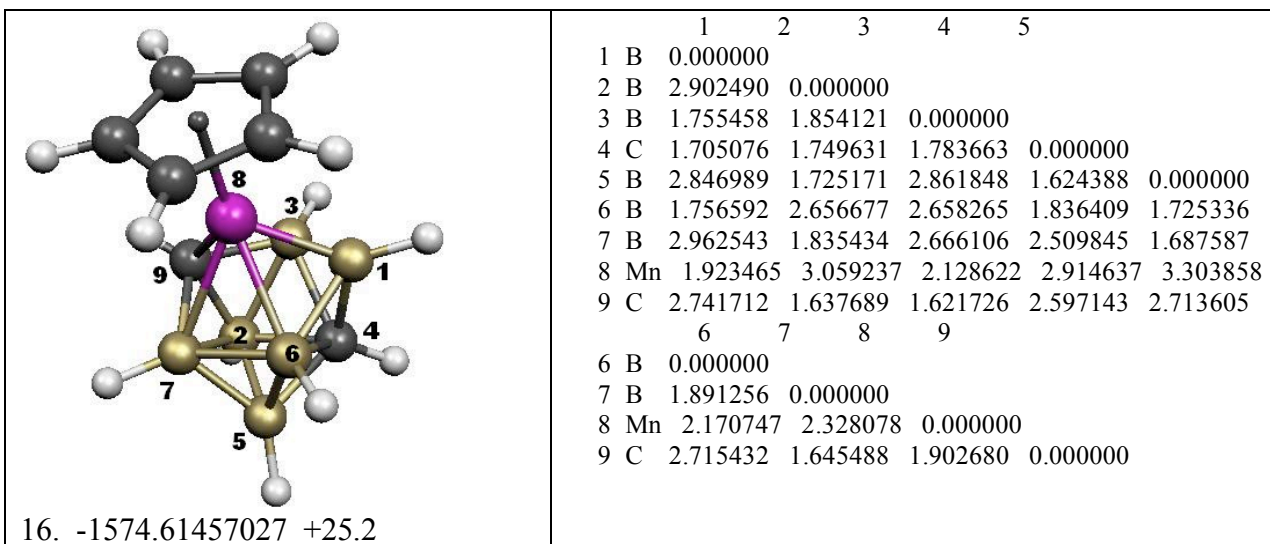


Table 3. Energy ranking

	Initial structure	Final energy (a.u.)	D kcal/mole	Remarks
1	1-CapCube_Mn_v5_C2_v43b	-1574.65469642	0.00	
2	3-Tl99-Mn_v6_C2_v44c	-1574.65469243	0.00	
3	2-PressCapCube_Mn_v5_C2_v44b	-1574.65469192	0.00	
4	1-CapCube_Mn_v4b_C2_v43g_r-24	-1574.65468229	0.01	
5	1-CapCube_Mn_v4b_C2_v43a	-1574.65468225	0.01	
6	1-CapCube_Mn_v5_C2_v43g_i-14	-1574.65464374	0.03	
7	1-CapCube_Mn_v4b_C2_v43g_i-24	-1574.65463113	0.04	
8	3-Tl99-Mn_v4_C2-w	-1574.65140139	2.07	
9	3-Tl99-Mn_v5a_C2_v44b_r-36	-1574.65140139	2.07	
10	4-TrTrPr_Mn_v4_C2_v55c_r-36	-1574.65140139	2.07	
11	1-CapCube_Mn_v5_C2_v43c	-1574.65140138	2.07	
12	3-Tl99-Mn_v6_C2_v44b	-1574.65140124	2.07	
13	1-CapCube_Mn_v5_C2_v34b	-1574.65140115	2.07	
14	2-PressCapCube_Mn_v5_C2_v44f	-1574.65139938	2.07	
15	1-CapCube_Mn_v4b_C2_v34	-1574.65128677	2.14	
16	4-TrTrPr_Mn_v4_C2_v55c_i-36	-1574.65071970	2.50	
17	3-Tl99-Mn_v5a_C2_v44b_i-36	-1574.65071931	2.50	
18	2-PressCapCube_Mn_v5_C2_v44g	-1574.64188329	8.04	
19	3-Tl99-Mn_v5b_C2_v55a	-1574.64188319	8.04	
20	3-Tl99-Mn_v6_C2_v45b	-1574.64188309	8.04	
21	1-CapCube_Mn_v5_C2_v44d	-1574.64188303	8.04	
22	1-CapCube_Mn_v4b_C2_v44g	-1574.64187694	8.04	
23	1-CapCube_Mn_v5_C2_v33d_i-25	-1574.64112716	8.51	
24	4-TrTrPr_Mn_v5_C2_v44a	-1574.63883303	9.95	
25	2-PressCapCube_Mn_v4_C2_v44b	-1574.63883295	9.95	
26	2-PressCapCube_Mn_v5_C2_v43a	-1574.63883294	9.95	
27	3-Tl99-Mn_v4_C2-g	-1574.63883294	9.95	
28	3-Tl99-Mn_v5a_C2_v54a	-1574.63883289	9.95	
29	4-TrTrPr_Mn_v4_C2_v55b	-1574.63883289	9.95	
30	3-Tl99-Mn_v5b_C2_v54c	-1574.63883285	9.95	
31	4-TrTrPr_Mn_v5_C2_v55b	-1574.63883277	9.95	
32	3-Tl99-Mn_v4_C2-k	-1574.63883262	9.95	
33	2-PressCapCube_Mn_v5_C2_v33	-1574.63883234	9.95	
34	2-PressCapCube_Mn_v4_C2_v54a	-1574.63883219	9.95	
35	3-Tl99-Mn_v4_C2-r	-1574.63883211	9.95	
36	2-PressCapCube_Mn_v5_C2_v44e	-1574.63883115	9.96	
37	3-Tl99-Mn_v5b_C2_v44b	-1574.63883097	9.96	
38	4-TrTrPr_Mn_v5_C2_v55e_r-37	-1574.63512084	12.28	

39	1-CapCube_Mn_v4_C2_v44b	-1574.63512069	12.28	
40	3-Tl99-Mn_v4_C2-b	-1574.63512067	12.28	
41	3-Tl99-Mn_v5b_C2_v45b	-1574.63512060	12.28	
42	2-PressCapCube_Mn_v4_C2_v54c	-1574.63512045	12.28	
43	4-TrTrPr_Mn_v5_C2_v44b	-1574.63512038	12.28	
44	1-CapCube_Mn_v4_C2_v44a	-1574.63512032	12.28	
45	4-TrTrPr_Mn_v5_C2_v55e i-37	-1574.63413545	12.90	
46	3-Tl99-Mn_v6_C2_v55c_r-28	-1574.62954536	15.78	
47	3-Tl99-Mn_v5a_C2_v65a_r-28	-1574.62954425	15.78	
48	3-Tl99-Mn_v5a_C2_v65a i-28	-1574.62948449	15.82	
49	3-Tl99-Mn_v6_C2_v55c i-28	-1574.62947583	15.83	C-C
50	3-Tl99-Mn_v6_C2_v44a_r-48	-1574.62754355	17.04	C-C
51	1-CapCube_Mn_v5_C2_v33c	-1574.62754352	17.04	C-C
52	1-CapCube_Mn_v5_C2_v44b	-1574.62754329	17.04	C-C
53	2-PressCapCube_Mn_v5_C2_v44c	-1574.62754329	17.04	C-C
54	2-PressCapCube_Mn_v5_C2_v43c_r-48	-1574.62754256	17.04	C-C
55	2-PressCapCube_Mn_v5_C2_v43c i-48	-1574.62583706	18.11	C-C
56	3-Tl99-Mn_v6_C2_v44a i-48	-1574.62583641	18.11	C-C
57	1-CapCube_Mn_v4b_C2_v44b	-1574.62405144	19.23	
58	1-CapCube_Mn_v4b_C2_v43d	-1574.62405143	19.23	
59	3-Tl99-Mn_v6_C2_v54b	-1574.62325636	19.73	
60	1-CapCube_Mn_v5_C2_v34a	-1574.62325611	19.73	
61	2-PressCapCube_Mn_v5_C2_v53	-1574.62325606	19.73	
62	2-PressCapCube_Mn_v5_C2_v54b_r-30	-1574.62324892	19.73	
63	2-PressCapCube_Mn_v5_C2_v54b i-30	-1574.62273663	20.05	
64	1-CapCube_Mn_v5_C2_v43f	-1574.62042106	21.51	
65	3-Tl99-Mn_v4_C2-f	-1574.61947993	22.10	
66	3-Tl99-Mn_v5b_C2_v55c	-1574.61947973	22.10	
67	3-Tl99-Mn_v5b_C2_v54a	-1574.61947966	22.10	
68	3-Tl99-Mn_v4_C2-n	-1574.61947885	22.10	
69	4-TrTrPr_Mn_v5_C2_v54c	-1574.61947805	22.10	
70	3-Tl99-Mn_v5a_C2_v45b	-1574.61947608	22.10	
71	1-CapCube_Mn_v4b_C2_v43b	-1574.61947506	22.10	
72	1-CapCube_Mn_v4_C2_v33a	-1574.61903538	22.38	
73	3-Tl99-Mn_v4_C2-y	-1574.61903536	22.38	
74	3-Tl99-Mn_v5b_C2_v65b Cs	-1574.61903532	22.38	
75	4-TrTrPr_Mn_v5_C2_v45	-1574.61903428	22.38	
76	1-CapCube_Mn_v5_C2_v43h	-1574.61597032	24.30	C-C
77	3-Tl99-Mn_v6_C2_v45a	-1574.61596956	24.30	C-C
78	2-PressCapCube_Mn_v4_C2_v43a	-1574.61596937	24.30	C-C
79	1-CapCube_Mn_v5_C2_v43e	-1574.61591057	24.34	

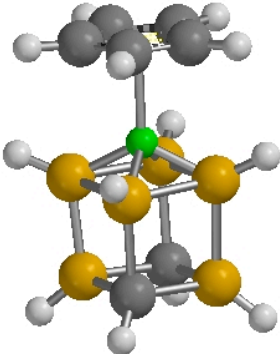
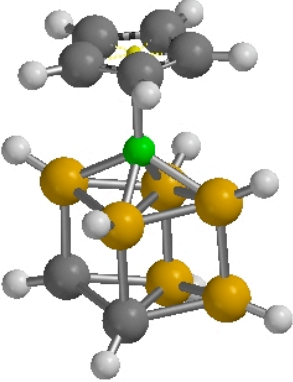
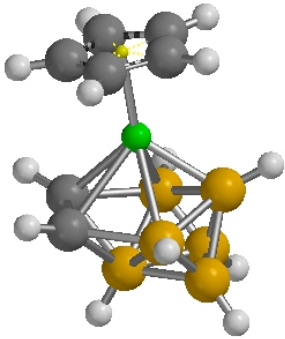
80	3-Tl99-Mn_v4_C2-e	-1574.61457027	25.18	
81	4-TrTrPr_Mn_v5_C2_v54f	-1574.61457019	25.18	
82	3-Tl99-Mn_v5b_C2_v44c	-1574.61457010	25.18	
83	3-Tl99-Mn_v4_C2-o	-1574.61456999	25.18	
84	3-Tl99-Mn_v5b_C2_v65a	-1574.61456998	25.18	
85	1-CapCube_Mn_v5_C2_v44a	-1574.61261614	26.41	C-C
86	3-Tl99-Mn_v5a_C2_v55	-1574.61135786	27.19	
87	1-CapCube_Mn_v4b_C2_v44f	-1574.61135735	27.20	
88	2-PressCapCube_Mn_v4_C2_v55	-1574.61043390	27.77	
89	1-CapCube_Mn_v4b_C2_v43c_r-24	-1574.60800520	29.30	
90	2-PressCapCube_Mn_v5_C2_v44a	-1574.60800511	29.30	
91	1-CapCube_Mn_v5_C2_v43a	-1574.60800311	29.30	
92	1-CapCube_Mn_v4b_C2_v43c_i-24	-1574.60757156	29.57	
93	1-CapCube_Mn_v4b_C2_v44c	-1574.60711945	29.85	C-C
94	3-Tl99-Mn_v5a_C2_v45a	-1574.60711853	29.86	C-C
95	4-TrTrPr_Mn_v5_C2_v54d	-1574.60365373	32.03	
96	3-Tl99-Mn_v4_C2-v	-1574.60365294	32.03	
97	4-TrTrPr_Mn_v4_C2_v44	-1574.60358824	32.07	
98	3-Tl99-Mn_v5a_C2_v44d	-1574.60358795	32.07	
99	1-CapCube_Mn_v4b_C2_v33b_r-36	-1574.60354762	32.10	
100	1-CapCube_Mn_v4b_C2_v33b_i-36	-1574.60216637	32.96	
101	2-PressCapCube_Mn_v4_C2_v33	-1574.60052331	33.99	
102	3-Tl99-Mn_v4_C2-i_r-30	-1574.60011749	34.25	
103	4-TrTrPr_Mn_v5_C2_v55a	-1574.60011710	34.25	
104	3-Tl99-Mn_v4_C2-i_-30	-1574.59959969	34.57	
105	1-CapCube_Mn_v5_C2_v33a	-1574.59952586	34.62	
106	2-PressCapCube_Mn_v5_C2_v45	-1574.59952567	34.62	
107	2-PressCapCube_Mn_v5_C2_v44d	-1574.59952544	34.62	C-C
108	3-Tl99-Mn_v6_C2_v54a	-1574.59952543	34.62	C-C
109	3-Tl99-Mn_v4_C2-d	-1574.59893865	34.99	C-C
110	1-CapCube_Mn_v4_C2_v34a	-1574.59893849	34.99	C-C
111	3-Tl99-Mn_v4_C2-q	-1574.59893839	34.99	C-C
112	4-TrTrPr_Mn_v5_C2_v54b	-1574.59893834	34.99	C-C
113	2-PressCapCube_Mn_v4_C2_v43b	-1574.59893807	34.99	C-C
114	2-PressCapCube_Mn_v5_C2_v54c	-1574.59761292	35.82	
115	3-Tl99-Mn_v4_C2-h	-1574.59616892	36.73	C-C
116	3-Tl99-Mn_v5b_C2_v45a	-1574.59616152	36.73	C-C
117	4-TrTrPr_Mn_v5_C2_v54a	-1574.59616061	36.73	C-C
118	3-Tl99-Mn_v5b_C2_v44a_r-303	-1574.59615008	36.74	C-C
119	2-PressCapCube_Mn_v4_C2_v54b	-1574.59395649	38.11	
120	3-Tl99-Mn_v4_C2-m_r-62	-1574.59395492	38.12	

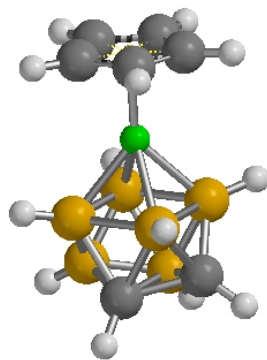
121	3-Tl99-Mn_v4_C2-s	-1574.59086620	40.05	
122	3-Tl99-Mn_v5a_C2_v54d	-1574.59086517	40.05	
123	3-Tl99-Mn_v4_C2-m	-1574.59085293	40.06	
124	1-CapCube_Mn_v5_C2_v44c	-1574.59066605	40.18	C-C
125	3-Tl99-Mn_v4_C2-j	-1574.59058686	40.23	C-C
126	4-TrTrPr_Mn_v5_C2_v45b	-1574.59058683	40.23	
127	3-Tl99-Mn_v5b_C2_v55b	-1574.59058669	40.23	C-C
128	3-Tl99-Mn_v4_C2-zz	-1574.59058648	40.23	C-C
129	3-Tl99-Mn_v4_C2-x	-1574.59058573	40.23	C-C
130	3-Tl99-Mn_v5b_C2_v64a	-1574.59058037	40.23	C-C
131	3-Tl99-Mn_v4_C2-p	-1574.59050929	40.28	C-C
132	2-PressCapCube_Mn_v5_C2_v43d	-1574.59050924	40.28	C-C
133	3-Tl99-Mn_v5b_C2_v54b	-1574.59050877	40.28	C-C
134	4-TrTrPr_Mn_v5_C2_v54e	-1574.59050621	40.28	C-C
135	4-TrTrPr_Mn_v5_C2_v55d	-1574.58982964	40.70	
136	2-PressCapCube_Mn_v4_C2_v43c_r-29	-1574.58876946	41.37	
137	2-PressCapCube_Mn_v4_C2_v44c	-1574.58876939	41.37	
138	1-CapCube_Mn_v4_C2_v34c	-1574.58876916	41.37	
139	3-Tl99-Mn_v6_C2_v55b	-1574.58833759	41.64	C-C
140	1-CapCube_Mn_v5_C2_v33b	-1574.58665937	42.69	
141	3-Tl99-Mn_v4_C2-zzz	-1574.58607582	43.06	C-C
142	3-Tl99-Mn_v5a_C2_v54b	-1574.58607576	43.06	C-C
143	2-PressCapCube_Mn_v5_C2_v43b	-1574.58607515	43.06	C-C
144	3-Tl99-Mn_v5b_C2_v44d_r-226	-1574.58607165	43.06	C-C
145	3-Tl99-Mn_v5b_C2_v64b	-1574.58606919	43.06	C-C
146	4-TrTrPr_Mn_v5_C2_v45c	-1574.58606293	43.07	
147	3-Tl99-Mn_v4_C2-t	-1574.58595203	43.14	C-C
148	1-CapCube_Mn_v4b_C2_v33a_r-21	-1574.58520931	43.60	
149	1-CapCube_Mn_v4b_C2_v33a_i-21	-1574.58426142	44.20	
150	1-CapCube_Mn_v4_C2_v34b	-1574.58370707	44.55	
151	2-PressCapCube_Mn_v4_C2_v53	-1574.58370701	44.55	
152	3-Tl99-Mn_v5a_C2_v44c	-1574.58370696	44.55	
153	1-CapCube_Mn_v4b_C2_v44a	-1574.58347538	44.69	C-C
154	1-CapCube_Mn_v4b_C2_v43f	-1574.58347060	44.69	
155	3-Tl99-Mn_v5a_C2_v64b	-1574.58298464	45.00	
156	1-CapCube_Mn_v5_C2_v43d	-1574.58048144	46.57	C-C
157	1-CapCube_Mn_v4b_C2_v44d	-1574.57336263	51.04	C-C
158	3-Tl99-Mn_v6_C2_v55a_r-20	-1574.57251853	51.57	
159	3-Tl99-Mn_v6_C2_v55a	-1574.57246913	51.60	
160	1-CapCube_Mn_v4b_C2_v43h	-1574.57196674	51.91	C-C
161	3-Tl99-Mn_v5a_C2_v64a	-1574.57077011	52.66	

162	3-Tl99-Mn_v4_C2-z	-1574.56897044	53.79	C-C
163	4-TrTrPr_Mn_v5_C2_v55c	-1574.56897016	53.79	C-C
164	3-Tl99-Mn_v4_C2-a	-1574.56706588	54.99	C-C
165	1-CapCube_Mn_v4b_C2_v44e	-1574.56634297	55.44	C-C
166	3-Tl99-Mn_v5b_C2_v44d i-226	-1574.56566078	55.87	C-C
167	3-Tl99-Mn_v4_C2-l	-1574.56549912	55.97	
168	2-PressCapCube_Mn_v5_C2_v54a	-1574.56452119	56.58	C-C
169	1-CapCube_Mn_v4b_C2_v43e	-1574.56396930	56.93	C-C
170	3-Tl99-Mn_v5b_C2_v44a i-303	-1574.56068104	58.99	C-C
171	4-TrTrPr_Mn_v4_C2_v55e	-1574.55823940	60.53	
172	3-Tl99-Mn_v5a_C2_v54c	-1574.55257402	64.08	C-C
173	3-Tl99-Mn_v4_C2-c	-1574.55257387	64.08	C-C
174	4-TrTrPr_Mn_v4_C2_v54b	-1574.55257194	64.08	C-C
175	3-Tl99-Mn_v5a_C2_v44a	-1574.55210221	64.38	C-C
176	4-TrTrPr_Mn_v4_C2_v54a	-1574.54911019	66.26	C-C
177	3-Tl99-Mn_v4_C2-u	-1574.54902684	66.31	C-C
178	2-PressCapCube_Mn_v4_C2_v43c i-29	-1574.54746267	67.29	
179	1-CapCube_Mn_v4_C2_v33b	-1574.54332587	69.89	C-C
180	3-Tl99-Mn_v5a_C2_v65b	-1574.53795250	73.26	
181	3-Tl99-Mn_v5a_C2_v55b i-19	-1574.52445402	81.73	
182	4-TrTrPr_Mn_v4_C2_v55d	-1574.52297191	82.66	C-C
183	2-PressCapCube_Mn_v4_C2_v44a	-1574.52232323	83.06	C-C
184	4-TrTrPr_Mn_v4_C2_v55a	-1574.51540455	87.41	

9-vertex $\text{CpReC}_2\text{B}_6\text{H}_8$

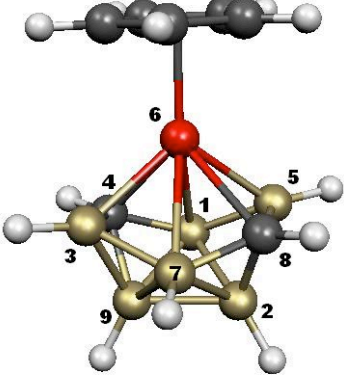
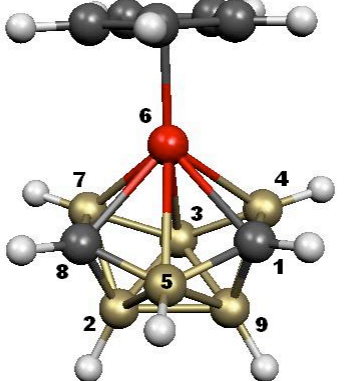
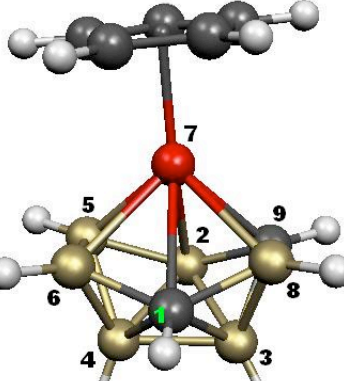
Table 1. Initial structures (one example from each family) 166 structures in total

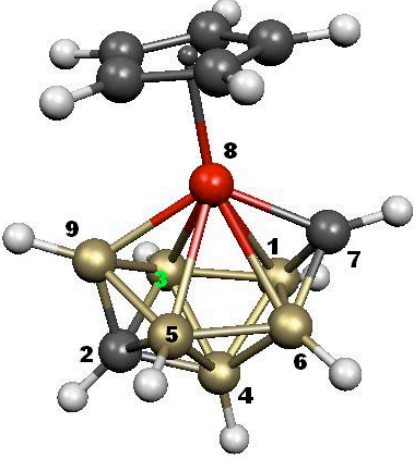
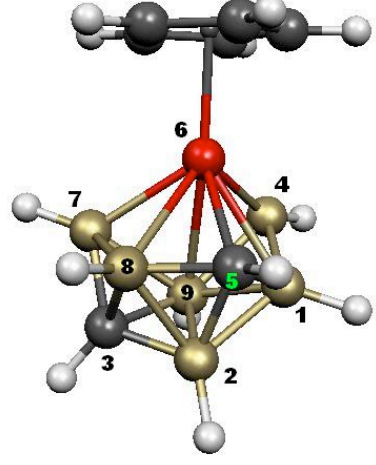
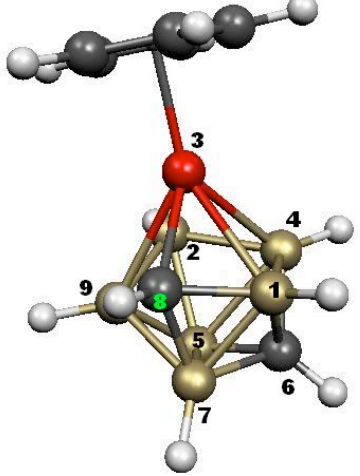
Initial structures
 <p>1. Capped cube 43 structures</p>
 <p>2. Pressed capped cube 29 structures</p>
 <p>3. Tl_9-like structure 70 structures</p>

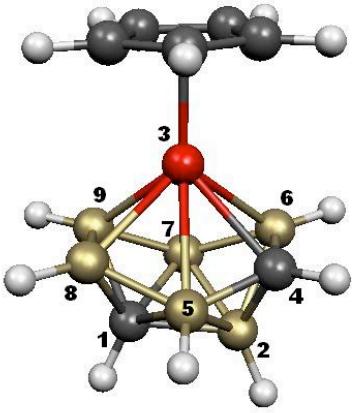
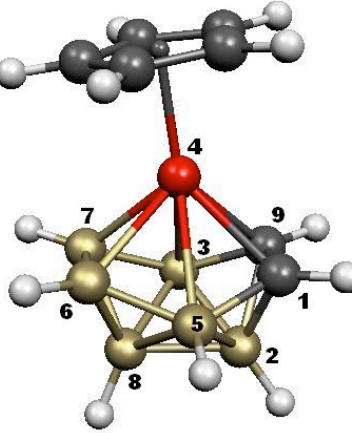
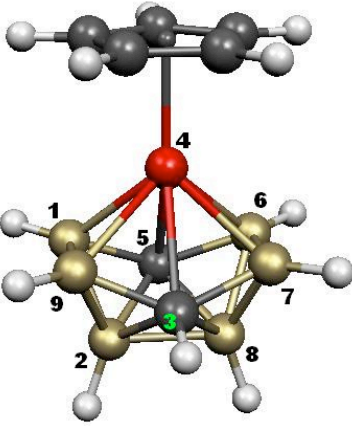


4. Tricapped trigonal prism 24 structures

Table 2. Distance table for the best structures

 <p>1. -502.08345088 0.0 C2</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.870533</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.734260</td><td>2.975722</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.591719</td><td>2.786067</td><td>1.590869</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.747795</td><td>1.823355</td><td>3.433954</td><td>2.911258</td><td>0.000000</td></tr> <tr><td>6 Re</td><td>2.386017</td><td>2.962372</td><td>2.151436</td><td>2.156165</td><td>2.154048</td></tr> <tr><td>7 B</td><td>2.752232</td><td>1.860589</td><td>1.749150</td><td>2.607761</td><td>2.733848</td></tr> <tr><td>8 C</td><td>2.606678</td><td>1.629961</td><td>2.912345</td><td>3.181618</td><td>1.590575</td></tr> <tr><td>9 B</td><td>1.859521</td><td>1.829025</td><td>1.823546</td><td>1.629724</td><td>2.974891</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>6 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.387373</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.161245</td><td>1.591313</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.960290</td><td>1.872243</td><td>2.786180</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.870533	0.000000				3 B	2.734260	2.975722	0.000000			4 C	1.591719	2.786067	1.590869	0.000000		5 B	1.747795	1.823355	3.433954	2.911258	0.000000	6 Re	2.386017	2.962372	2.151436	2.156165	2.154048	7 B	2.752232	1.860589	1.749150	2.607761	2.733848	8 C	2.606678	1.629961	2.912345	3.181618	1.590575	9 B	1.859521	1.829025	1.823546	1.629724	2.974891		6	7	8	9		6 Re	0.000000					7 B	2.387373	0.000000				8 C	2.161245	1.591313	0.000000			9 B	2.960290	1.872243	2.786180	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.870533	0.000000																																																																																									
3 B	2.734260	2.975722	0.000000																																																																																								
4 C	1.591719	2.786067	1.590869	0.000000																																																																																							
5 B	1.747795	1.823355	3.433954	2.911258	0.000000																																																																																						
6 Re	2.386017	2.962372	2.151436	2.156165	2.154048																																																																																						
7 B	2.752232	1.860589	1.749150	2.607761	2.733848																																																																																						
8 C	2.606678	1.629961	2.912345	3.181618	1.590575																																																																																						
9 B	1.859521	1.829025	1.823546	1.629724	2.974891																																																																																						
	6	7	8	9																																																																																							
6 Re	0.000000																																																																																										
7 B	2.387373	0.000000																																																																																									
8 C	2.161245	1.591313	0.000000																																																																																								
9 B	2.960290	1.872243	2.786180	0.000000																																																																																							
 <p>2. -502.07847026 +3.1 Cs</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.806323</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.591184</td><td>1.821415</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.595328</td><td>2.955706</td><td>1.719961</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.610382</td><td>1.900786</td><td>2.748648</td><td>2.748706</td><td>0.000000</td></tr> <tr><td>6 Re</td><td>2.125790</td><td>2.965171</td><td>2.440025</td><td>2.188458</td><td>2.364449</td></tr> <tr><td>7 B</td><td>3.298787</td><td>1.782821</td><td>1.719961</td><td>2.994800</td><td>2.748706</td></tr> <tr><td>8 C</td><td>2.783800</td><td>1.645986</td><td>2.591184</td><td>3.298787</td><td>1.610382</td></tr> <tr><td>9 B</td><td>1.645986</td><td>1.855800</td><td>1.821415</td><td>1.782821</td><td>1.900786</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>6 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.188458</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.125790</td><td>1.595328</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.965171</td><td>2.955706</td><td>2.806323</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	2.806323	0.000000				3 B	2.591184	1.821415	0.000000			4 B	1.595328	2.955706	1.719961	0.000000		5 B	1.610382	1.900786	2.748648	2.748706	0.000000	6 Re	2.125790	2.965171	2.440025	2.188458	2.364449	7 B	3.298787	1.782821	1.719961	2.994800	2.748706	8 C	2.783800	1.645986	2.591184	3.298787	1.610382	9 B	1.645986	1.855800	1.821415	1.782821	1.900786		6	7	8	9		6 Re	0.000000					7 B	2.188458	0.000000				8 C	2.125790	1.595328	0.000000			9 B	2.965171	2.955706	2.806323	0.000000	
	1	2	3	4	5																																																																																						
1 C	0.000000																																																																																										
2 B	2.806323	0.000000																																																																																									
3 B	2.591184	1.821415	0.000000																																																																																								
4 B	1.595328	2.955706	1.719961	0.000000																																																																																							
5 B	1.610382	1.900786	2.748648	2.748706	0.000000																																																																																						
6 Re	2.125790	2.965171	2.440025	2.188458	2.364449																																																																																						
7 B	3.298787	1.782821	1.719961	2.994800	2.748706																																																																																						
8 C	2.783800	1.645986	2.591184	3.298787	1.610382																																																																																						
9 B	1.645986	1.855800	1.821415	1.782821	1.900786																																																																																						
	6	7	8	9																																																																																							
6 Re	0.000000																																																																																										
7 B	2.188458	0.000000																																																																																									
8 C	2.125790	1.595328	0.000000																																																																																								
9 B	2.965171	2.955706	2.806323	0.000000																																																																																							
 <p>3. -502.07007137 +8.4</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.599478</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.736996</td><td>1.840772</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.775073</td><td>1.880909</td><td>1.833873</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.635585</td><td>1.754248</td><td>2.946394</td><td>1.763871</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.634385</td><td>2.767289</td><td>2.905321</td><td>1.755550</td><td>1.704600</td></tr> <tr><td>7 Re</td><td>2.313106</td><td>2.362314</td><td>2.954916</td><td>2.938085</td><td>2.167053</td></tr> <tr><td>8 B</td><td>1.641184</td><td>2.717453</td><td>1.818236</td><td>2.960944</td><td>3.431912</td></tr> <tr><td>9 C</td><td>2.461468</td><td>1.602097</td><td>1.631225</td><td>2.808646</td><td>2.946051</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 Re</td><td>2.192018</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.952111</td><td>2.167274</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.313391</td><td>2.165602</td><td>1.582668</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	2.599478	0.000000				3 B	1.736996	1.840772	0.000000			4 B	1.775073	1.880909	1.833873	0.000000		5 B	2.635585	1.754248	2.946394	1.763871	0.000000	6 B	1.634385	2.767289	2.905321	1.755550	1.704600	7 Re	2.313106	2.362314	2.954916	2.938085	2.167053	8 B	1.641184	2.717453	1.818236	2.960944	3.431912	9 C	2.461468	1.602097	1.631225	2.808646	2.946051		6	7	8	9		6 B	0.000000					7 Re	2.192018	0.000000				8 B	2.952111	2.167274	0.000000			9 C	3.313391	2.165602	1.582668	0.000000	
	1	2	3	4	5																																																																																						
1 C	0.000000																																																																																										
2 B	2.599478	0.000000																																																																																									
3 B	1.736996	1.840772	0.000000																																																																																								
4 B	1.775073	1.880909	1.833873	0.000000																																																																																							
5 B	2.635585	1.754248	2.946394	1.763871	0.000000																																																																																						
6 B	1.634385	2.767289	2.905321	1.755550	1.704600																																																																																						
7 Re	2.313106	2.362314	2.954916	2.938085	2.167053																																																																																						
8 B	1.641184	2.717453	1.818236	2.960944	3.431912																																																																																						
9 C	2.461468	1.602097	1.631225	2.808646	2.946051																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 Re	2.192018	0.000000																																																																																									
8 B	2.952111	2.167274	0.000000																																																																																								
9 C	3.313391	2.165602	1.582668	0.000000																																																																																							

 <p>4. -502.06837673 +9.5 Cs</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 C</td><td>2.787130</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.804781</td><td>1.670146</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.795713</td><td>1.579953</td><td>1.918179</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.792781</td><td>1.670146</td><td>2.503800</td><td>1.918179</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.814200</td><td>2.787130</td><td>2.792781</td><td>1.795713</td><td>1.804781</td></tr> <tr><td>7 C</td><td>1.592498</td><td>3.703170</td><td>2.940912</td><td>2.848102</td><td>2.940912</td></tr> <tr><td>8 Re</td><td>2.398444</td><td>3.040113</td><td>2.353709</td><td>3.112056</td><td>2.353709</td></tr> <tr><td>9 B</td><td>3.104153</td><td>1.552187</td><td>1.809161</td><td>2.691736</td><td>1.809161</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 C</td><td>1.592498</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Re</td><td>2.398444</td><td>1.935707</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.104153</td><td>3.553155</td><td>2.124007</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	2.787130	0.000000				3 B	1.804781	1.670146	0.000000			4 B	1.795713	1.579953	1.918179	0.000000		5 B	2.792781	1.670146	2.503800	1.918179	0.000000	6 B	1.814200	2.787130	2.792781	1.795713	1.804781	7 C	1.592498	3.703170	2.940912	2.848102	2.940912	8 Re	2.398444	3.040113	2.353709	3.112056	2.353709	9 B	3.104153	1.552187	1.809161	2.691736	1.809161		6	7	8	9		6 B	0.000000					7 C	1.592498	0.000000				8 Re	2.398444	1.935707	0.000000			9 B	3.104153	3.553155	2.124007	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 C	2.787130	0.000000																																																																																									
3 B	1.804781	1.670146	0.000000																																																																																								
4 B	1.795713	1.579953	1.918179	0.000000																																																																																							
5 B	2.792781	1.670146	2.503800	1.918179	0.000000																																																																																						
6 B	1.814200	2.787130	2.792781	1.795713	1.804781																																																																																						
7 C	1.592498	3.703170	2.940912	2.848102	2.940912																																																																																						
8 Re	2.398444	3.040113	2.353709	3.112056	2.353709																																																																																						
9 B	3.104153	1.552187	1.809161	2.691736	1.809161																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 C	1.592498	0.000000																																																																																									
8 Re	2.398444	1.935707	0.000000																																																																																								
9 B	3.104153	3.553155	2.124007	0.000000																																																																																							
 <p>5. -502.06428905 +12.0</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.815437</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.811354</td><td>1.597728</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.799663</td><td>3.162906</td><td>3.361850</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>1.581733</td><td>1.695571</td><td>2.600997</td><td>2.928749</td><td>0.000000</td></tr> <tr><td>6 Re</td><td>2.317649</td><td>3.096777</td><td>3.012171</td><td>1.990149</td><td>2.155291</td></tr> <tr><td>7 B</td><td>3.149195</td><td>2.719568</td><td>1.544258</td><td>3.021944</td><td>2.864065</td></tr> <tr><td>8 B</td><td>2.713500</td><td>1.866207</td><td>1.695698</td><td>3.567748</td><td>1.594562</td></tr> <tr><td>9 B</td><td>1.849925</td><td>1.884993</td><td>1.668349</td><td>1.851954</td><td>2.576974</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th></th> </tr> <tr><td>6 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.138495</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.379199</td><td>1.860493</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.435823</td><td>1.974959</td><td>2.576456</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.815437	0.000000				3 C	2.811354	1.597728	0.000000			4 B	1.799663	3.162906	3.361850	0.000000		5 C	1.581733	1.695571	2.600997	2.928749	0.000000	6 Re	2.317649	3.096777	3.012171	1.990149	2.155291	7 B	3.149195	2.719568	1.544258	3.021944	2.864065	8 B	2.713500	1.866207	1.695698	3.567748	1.594562	9 B	1.849925	1.884993	1.668349	1.851954	2.576974		6	7	8	9		6 Re	0.000000					7 B	2.138495	0.000000				8 B	2.379199	1.860493	0.000000			9 B	2.435823	1.974959	2.576456	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.815437	0.000000																																																																																									
3 C	2.811354	1.597728	0.000000																																																																																								
4 B	1.799663	3.162906	3.361850	0.000000																																																																																							
5 C	1.581733	1.695571	2.600997	2.928749	0.000000																																																																																						
6 Re	2.317649	3.096777	3.012171	1.990149	2.155291																																																																																						
7 B	3.149195	2.719568	1.544258	3.021944	2.864065																																																																																						
8 B	2.713500	1.866207	1.695698	3.567748	1.594562																																																																																						
9 B	1.849925	1.884993	1.668349	1.851954	2.576974																																																																																						
	6	7	8	9																																																																																							
6 Re	0.000000																																																																																										
7 B	2.138495	0.000000																																																																																									
8 B	2.379199	1.860493	0.000000																																																																																								
9 B	2.435823	1.974959	2.576456	0.000000																																																																																							
 <p>6. -502.06169161 +13.7</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>3.046252</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>2.367509</td><td>1.994073</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.838476</td><td>1.965332</td><td>2.209218</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.668540</td><td>1.918889</td><td>3.182648</td><td>2.131455</td><td>0.000000</td></tr> <tr><td>6 C</td><td>1.628600</td><td>2.791599</td><td>3.219743</td><td>1.618861</td><td>1.592338</td></tr> <tr><td>7 B</td><td>1.833015</td><td>3.025486</td><td>3.195943</td><td>2.710099</td><td>1.808979</td></tr> <tr><td>8 C</td><td>1.666002</td><td>2.823381</td><td>2.042869</td><td>2.771046</td><td>2.726781</td></tr> <tr><td>9 B</td><td>2.683155</td><td>1.827081</td><td>2.358548</td><td>2.772993</td><td>1.770463</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th></th> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.634947</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.607693</td><td>1.651090</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.666483</td><td>1.838944</td><td>1.669722</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.046252	0.000000				3 Re	2.367509	1.994073	0.000000			4 B	1.838476	1.965332	2.209218	0.000000		5 B	2.668540	1.918889	3.182648	2.131455	0.000000	6 C	1.628600	2.791599	3.219743	1.618861	1.592338	7 B	1.833015	3.025486	3.195943	2.710099	1.808979	8 C	1.666002	2.823381	2.042869	2.771046	2.726781	9 B	2.683155	1.827081	2.358548	2.772993	1.770463		6	7	8	9		6 C	0.000000					7 B	1.634947	0.000000				8 C	2.607693	1.651090	0.000000			9 B	2.666483	1.838944	1.669722	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	3.046252	0.000000																																																																																									
3 Re	2.367509	1.994073	0.000000																																																																																								
4 B	1.838476	1.965332	2.209218	0.000000																																																																																							
5 B	2.668540	1.918889	3.182648	2.131455	0.000000																																																																																						
6 C	1.628600	2.791599	3.219743	1.618861	1.592338																																																																																						
7 B	1.833015	3.025486	3.195943	2.710099	1.808979																																																																																						
8 C	1.666002	2.823381	2.042869	2.771046	2.726781																																																																																						
9 B	2.683155	1.827081	2.358548	2.772993	1.770463																																																																																						
	6	7	8	9																																																																																							
6 C	0.000000																																																																																										
7 B	1.634947	0.000000																																																																																									
8 C	2.607693	1.651090	0.000000																																																																																								
9 B	2.666483	1.838944	1.669722	0.000000																																																																																							

 <p>7. -502.05876141 +15.5</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.764675</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>2.798930</td><td>2.964995</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>2.686544</td><td>1.644448</td><td>2.182783</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.808376</td><td>1.868964</td><td>2.354414</td><td>1.579483</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.848112</td><td>1.787901</td><td>2.209250</td><td>1.573209</td><td>2.706219</td></tr> <tr><td>7 B</td><td>1.759641</td><td>1.797553</td><td>2.405856</td><td>2.574333</td><td>2.728827</td></tr> <tr><td>8 B</td><td>1.705678</td><td>2.943836</td><td>2.156344</td><td>2.913129</td><td>1.718256</td></tr> <tr><td>9 B</td><td>1.683933</td><td>2.913404</td><td>2.174339</td><td>3.317125</td><td>2.757478</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>1.712932</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.445875</td><td>2.756652</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.007024</td><td>1.708033</td><td>1.710225</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.764675	0.000000				3 Re	2.798930	2.964995	0.000000			4 C	2.686544	1.644448	2.182783	0.000000		5 B	1.808376	1.868964	2.354414	1.579483	0.000000	6 B	2.848112	1.787901	2.209250	1.573209	2.706219	7 B	1.759641	1.797553	2.405856	2.574333	2.728827	8 B	1.705678	2.943836	2.156344	2.913129	1.718256	9 B	1.683933	2.913404	2.174339	3.317125	2.757478		6	7	8	9		6 B	0.000000					7 B	1.712932	0.000000				8 B	3.445875	2.756652	0.000000			9 B	3.007024	1.708033	1.710225	0.000000	
	1	2	3	4	5																																																																																						
1 C	0.000000																																																																																										
2 B	1.764675	0.000000																																																																																									
3 Re	2.798930	2.964995	0.000000																																																																																								
4 C	2.686544	1.644448	2.182783	0.000000																																																																																							
5 B	1.808376	1.868964	2.354414	1.579483	0.000000																																																																																						
6 B	2.848112	1.787901	2.209250	1.573209	2.706219																																																																																						
7 B	1.759641	1.797553	2.405856	2.574333	2.728827																																																																																						
8 B	1.705678	2.943836	2.156344	2.913129	1.718256																																																																																						
9 B	1.683933	2.913404	2.174339	3.317125	2.757478																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 B	1.712932	0.000000																																																																																									
8 B	3.445875	2.756652	0.000000																																																																																								
9 B	3.007024	1.708033	1.710225	0.000000																																																																																							
 <p>8. -502.05748495 +16.3 Cs</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.699137</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.564767</td><td>1.836736</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Re</td><td>2.150096</td><td>2.998762</td><td>2.386618</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.588898</td><td>1.836886</td><td>2.728301</td><td>2.387353</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.913876</td><td>2.947936</td><td>2.772796</td><td>2.181737</td><td>1.739121</td></tr> <tr><td>7 B</td><td>3.321135</td><td>2.948503</td><td>1.739737</td><td>2.180350</td><td>2.772853</td></tr> <tr><td>8 B</td><td>2.823481</td><td>1.829415</td><td>1.883777</td><td>2.945111</td><td>1.883291</td></tr> <tr><td>9 C</td><td>1.485000</td><td>1.697864</td><td>1.589259</td><td>2.150640</td><td>2.564247</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>1.709102</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.766987</td><td>1.768231</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.321414</td><td>2.914623</td><td>2.823358</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.699137	0.000000				3 B	2.564767	1.836736	0.000000			4 Re	2.150096	2.998762	2.386618	0.000000		5 B	1.588898	1.836886	2.728301	2.387353	0.000000	6 B	2.913876	2.947936	2.772796	2.181737	1.739121	7 B	3.321135	2.948503	1.739737	2.180350	2.772853	8 B	2.823481	1.829415	1.883777	2.945111	1.883291	9 C	1.485000	1.697864	1.589259	2.150640	2.564247		6	7	8	9		6 B	0.000000					7 B	1.709102	0.000000				8 B	1.766987	1.768231	0.000000			9 C	3.321414	2.914623	2.823358	0.000000	
	1	2	3	4	5																																																																																						
1 C	0.000000																																																																																										
2 B	1.699137	0.000000																																																																																									
3 B	2.564767	1.836736	0.000000																																																																																								
4 Re	2.150096	2.998762	2.386618	0.000000																																																																																							
5 B	1.588898	1.836886	2.728301	2.387353	0.000000																																																																																						
6 B	2.913876	2.947936	2.772796	2.181737	1.739121																																																																																						
7 B	3.321135	2.948503	1.739737	2.180350	2.772853																																																																																						
8 B	2.823481	1.829415	1.883777	2.945111	1.883291																																																																																						
9 C	1.485000	1.697864	1.589259	2.150640	2.564247																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 B	1.709102	0.000000																																																																																									
8 B	1.766987	1.768231	0.000000																																																																																								
9 C	3.321414	2.914623	2.823358	0.000000																																																																																							
 <p>9. -502.05705076 +16.6 C2v</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.750091</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.622397</td><td>1.751855</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Re</td><td>2.187450</td><td>2.929757</td><td>2.296918</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>1.650106</td><td>1.752272</td><td>2.454200</td><td>2.297064</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.988800</td><td>2.935813</td><td>2.622397</td><td>2.187450</td><td>1.650106</td></tr> <tr><td>7 B</td><td>3.434888</td><td>2.935859</td><td>1.649344</td><td>2.186842</td><td>2.623362</td></tr> <tr><td>8 B</td><td>2.935813</td><td>1.859000</td><td>1.751855</td><td>2.929757</td><td>1.752272</td></tr> <tr><td>9 B</td><td>1.694201</td><td>1.751018</td><td>1.649344</td><td>2.186842</td><td>2.623362</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>1.694201</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.750091</td><td>1.751018</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.434888</td><td>2.987200</td><td>2.935859</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.750091	0.000000				3 C	2.622397	1.751855	0.000000			4 Re	2.187450	2.929757	2.296918	0.000000		5 C	1.650106	1.752272	2.454200	2.297064	0.000000	6 B	2.988800	2.935813	2.622397	2.187450	1.650106	7 B	3.434888	2.935859	1.649344	2.186842	2.623362	8 B	2.935813	1.859000	1.751855	2.929757	1.752272	9 B	1.694201	1.751018	1.649344	2.186842	2.623362		6	7	8	9		6 B	0.000000					7 B	1.694201	0.000000				8 B	1.750091	1.751018	0.000000			9 B	3.434888	2.987200	2.935859	0.000000	
	1	2	3	4	5																																																																																						
1 B	0.000000																																																																																										
2 B	1.750091	0.000000																																																																																									
3 C	2.622397	1.751855	0.000000																																																																																								
4 Re	2.187450	2.929757	2.296918	0.000000																																																																																							
5 C	1.650106	1.752272	2.454200	2.297064	0.000000																																																																																						
6 B	2.988800	2.935813	2.622397	2.187450	1.650106																																																																																						
7 B	3.434888	2.935859	1.649344	2.186842	2.623362																																																																																						
8 B	2.935813	1.859000	1.751855	2.929757	1.752272																																																																																						
9 B	1.694201	1.751018	1.649344	2.186842	2.623362																																																																																						
	6	7	8	9																																																																																							
6 B	0.000000																																																																																										
7 B	1.694201	0.000000																																																																																									
8 B	1.750091	1.751018	0.000000																																																																																								
9 B	3.434888	2.987200	2.935859	0.000000																																																																																							

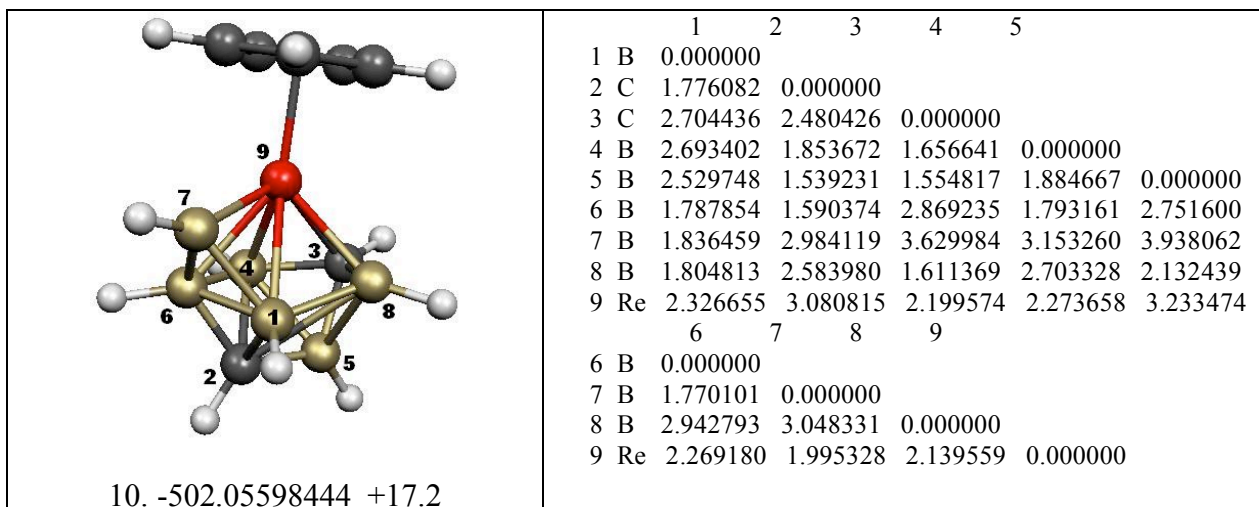


Table 3. Energy ranking

No	Initial structure	Final energy (a.u.)	ΔE kcal/mole	Remarks
1	1-CapCube_Re_v4b_C2_v43a	-502.08345088	0.00	
2	2-PressCapCube_Re_v5_C2_v44b	-502.08345087	0.00	
3	3-Tl99-Re_v4_C2-n	-502.08345087	0.00	
4	3-Tl99-Re_v6_C2_v44c	-502.08345087	0.00	
5	1-CapCube_Re_v5_C2_v43b	-502.08345086	0.00	
6	1-CapCube_Re_v4b_C2_v34	-502.07847026	3.13	
7	1-CapCube_Re_v5_C2_v34b	-502.07847026	3.13	
8	2-PressCapCube_Re_v5_C2_v43a	-502.07847026	3.13	
9	3-Tl99-Re_v5a_C2_v44b	-502.07847026	3.13	
10	3-Tl99-Re_v6_C2_v44b_r-29	-502.07847026	3.13	
11	4-TrTrPr_Re_v4_C2_v55c	-502.07847026	3.13	
12	4-TrTrPr_Re_v5_C2_v44b_r-58	-502.07847026	3.13	
13	4-TrTrPr_Re_v5_C2_v55e	-502.07847026	3.13	
14	3-Tl99-Re_v6_C2_v44b i-29	-502.07748343	3.74	
15	3-Tl99-Re_v6_C2_v45b	-502.07007137	8.40	
16	2-PressCapCube_Re_v5_C2_v44g	-502.07007136	8.40	
17	1-CapCube_Re_v4b_C2_v44g	-502.06997779	8.45	
18	2-PressCapCube_Re_v5_C2_v44f	-502.06997779	8.45	
19	1-CapCube_Re_v5_C2_v43c	-502.06997778	8.45	
20	1-CapCube_Re_v5_C2_v33d	-502.06997776	8.45	
21	1-CapCube_Re_v5_C2_v44d	-502.06995455	8.47	
22	2-PressCapCube_Re_v5_C2_v33	-502.06995455	8.47	
23	3-Tl99-Re_v4_C2-s_r-25	-502.06837673	9.46	
24	3-Tl99-Re_v4_C2-s i-25	-502.06825626	9.53	
25	1-CapCube_Re_v4b_C2_v43g	-502.06428905	12.02	
26	1-CapCube_Re_v4b_C2_v44b	-502.06428905	12.02	
27	1-CapCube_Re_v5_C2_v34a	-502.06428905	12.02	
28	1-CapCube_Re_v4b_C2_v43d	-502.06428904	12.02	
29	2-PressCapCube_Re_v4_C2_v44b	-502.06169165	13.65	
30	1-CapCube_Re_v4_C2_v34b	-502.06169164	13.65	
31	3-Tl99-Re_v4_C2-e	-502.06169164	13.65	
32	3-Tl99-Re_v5b_C2_v44c	-502.06169164	13.65	
33	4-TrTrPr_Re_v4_C2_v55b	-502.06169164	13.65	
34	3-Tl99-Re_v4_C2-o	-502.06169163	13.65	

35	4-TrTrPr_Re_v5_C2_v54f	-502.06169163	13.65	
36	4-TrTrPr_Re_v5_C2_v55c	-502.06169163	13.65	
37	3-Tl99-Re_v5a_C2_v44c	-502.06169162	13.65	
38	3-Tl99-Re_v5b_C2_v54c	-502.06169162	13.65	
39	3-Tl99-Re_v5b_C2_v65a	-502.06169162	13.65	
40	3-Tl99-Re_v5b_C2_v44b	-502.06169161	13.65	
41	2- PressCapCube_Re_v5_C2_v54b	-502.05876141	15.49	
42	1-CapCube_Re_v5_C2_v43f	-502.05876140	15.49	
43	3-Tl99-Re_v6_C2_v54b	-502.05876140	15.49	
44	1-CapCube_Re_v5_C2_v44b	-502.05748495	16.29	C-C
45	2- PressCapCube_Re_v5_C2_v43c	-502.05748495	16.29	C-C
46	3-Tl99-Re_v4_C2-q	-502.05748495	16.29	C-C
47	3-Tl99-Re_v6_C2_v44a	-502.05718102	16.48	C-C
48	1-CapCube_Re_v5_C2_v43g	-502.05705076	16.57	
49	3-Tl99-Re_v6_C2_v55c	-502.05697673	16.61	
50	2- PressCapCube_Re_v4_C2_v54b	-502.05598444	17.24	
51	1-CapCube_Re_v4b_C2_v44f	-502.05598443	17.24	
52	2-PressCapCube_Re_v5_C2_v53	-502.05328354	18.93	
53	1-CapCube_Re_v5_C2_v43a	-502.05328352	18.93	
54	1-CapCube_Re_v4b_C2_v43c	-502.05328351	18.93	
55	2- PressCapCube_Re_v5_C2_v44a	-502.05328348	18.93	
56	1-CapCube_Re_v4_C2_v34a	-502.05239426	19.49	C-C
57	2- PressCapCube_Re_v4_C2_v43c	-502.05061027	20.61	
58	3-Tl99-Re_v5a_C2_v54d	-502.05061027	20.61	
59	1-CapCube_Re_v4b_C2_v43b	-502.05050033	20.68	
60	1-CapCube_Re_v4b_C2_v44c	-502.04802143	22.23	C-C
61	1-CapCube_Re_v4_C2_v34c	-502.04650677	23.18	
62	4-TrTrPr_Re_v4_C2_v55e	-502.04650676	23.18	
63	1-CapCube_Re_v4b_C2_v43h	-502.04363739	24.98	C-C
64	1-CapCube_Re_v5_C2_v33c	-502.04363739	24.98	C-C
65	2- PressCapCube_Re_v5_C2_v43d	-502.04363739	24.98	C-C
66	3-Tl99-Re_v5a_C2_v55	-502.04363739	24.98	C-C
67	3-Tl99-Re_v6_C2_v45a	-502.04363739	24.98	C-C
68	1-CapCube_Re_v5_C2_v43h	-502.04363738	24.98	C-C
69	3-Tl99-Re_v4_C2-h	-502.04363738	24.98	C-C
70	4-TrTrPr_Re_v5_C2_v45b	-502.04363738	24.98	C-C
71	1-CapCube_Re_v4_C2_v44a	-502.04358019	25.02	

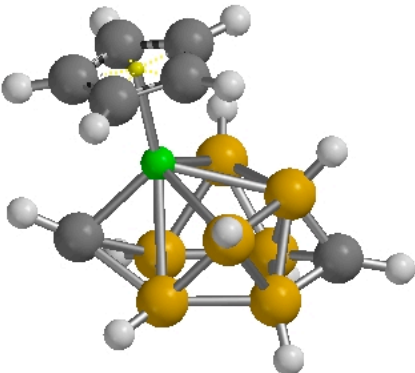
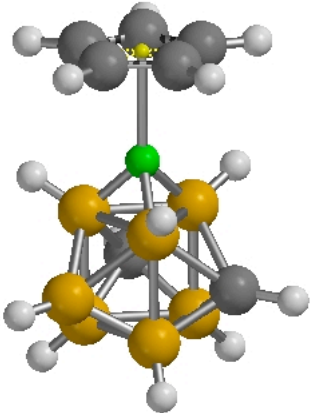
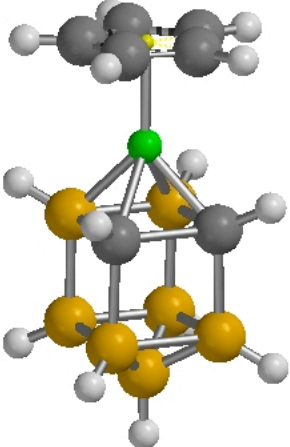
72	1-CapCube_Re_v4_C2_v44b	-502.04358019	25.02	
73	3-Tl99-Re_v5b_C2_v45b	-502.04358019	25.02	
74	3-Tl99-Re_v5b_C2_v55c_r-22	-502.04358019	25.02	
75	3-Tl99-Re_v5b_C2_v55c_i-22	-502.04337244	25.15	
76	3-Tl99-Re_v5a_C2_v54a	-502.04131892	26.44	
77	3-Tl99-Re_v4_C2-g	-502.04131891	26.44	
78	3-Tl99-Re_v4_C2-r	-502.04131891	26.44	
79	4-TrTrPr_Re_v5_C2_v44a	-502.04131891	26.44	
80	4-TrTrPr_Re_v5_C2_v55d	-502.03884102	27.99	
81	3-Tl99-Re_v5b_C2_v65b	-502.03880821	28.01	
82	1-CapCube_Re_v4b_C2_v33b	-502.03865489	28.11	
83	3-Tl99-Re_v5a_C2_v45a	-502.03865489	28.11	
84	3-Tl99-Re_v4_C2-p	-502.03335003	31.44	C-C
85	1-CapCube_Re_v5_C2_v44a	-502.03335002	31.44	C-C
86	2-PressCapCube_Re_v5_C2_v43b	-502.03335002	31.44	C-C
87	1-CapCube_Re_v5_C2_v33b	-502.03335001	31.44	C-C
88	1-CapCube_Re_v5_C2_v44c	-502.03335001	31.44	C-C
89	2-PressCapCube_Re_v5_C2_v44d	-502.03335001	31.44	C-C
90	2-PressCapCube_Re_v5_C2_v45	-502.03335001	31.44	C-C
91	2-PressCapCube_Re_v5_C2_v54c	-502.03335001	31.44	C-C
92	3-Tl99-Re_v6_C2_v54a	-502.03335001	31.44	C-C
93	3-Tl99-Re_v4_C2-v	-502.03290370	31.72	
94	3-Tl99-Re_v5a_C2_v45b	-502.03192312	32.33	
95	3-Tl99-Re_v5b_C2_v54a	-502.03192312	32.33	
96	4-TrTrPr_Re_v5_C2_v54c	-502.03192312	32.33	
97	4-TrTrPr_Re_v4_C2_v54a	-502.02836387	34.57	C-C
98	4-TrTrPr_Re_v5_C2_v45c	-502.02836387	34.57	C-C
99	1-CapCube_Re_v4b_C2_v43f	-502.02726223	35.26	C-C
100	1-CapCube_Re_v4b_C2_v44a	-502.02726223	35.26	C-C
101	2-PressCapCube_Re_v4_C2_v33	-502.02695444	35.45	
102	3-Tl99-Re_v5a_C2_v65a	-502.02641671	35.79	
103	4-TrTrPr_Re_v5_C2_v45_r-26	-502.02641663	35.79	
104	4-TrTrPr_Re_v5_C2_v45_r-103	-502.02641662	35.79	
105	1-CapCube_Re_v5_C2_v33a	-502.02384796	37.40	C-C
106	1-CapCube_Re_v5_C2_v43e	-502.02384796	37.40	C-C
107	3-Tl99-Re_v6_C2_v55b	-502.02384796	37.40	C-C
108	2-PressCapCube_Re_v5_C2_v44c	-502.02187668	38.64	C-C
109	1-CapCube_Re_v4_C2_v33a	-502.02175444	38.71	

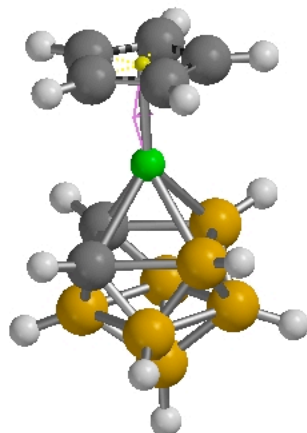
110	1-CapCube_Re_v5_C2_v43d	-502.01981407	39.93	
111	2-PressCapCube_Re_v5_C2_v54a	-502.01981407	39.93	
112	3-Tl99-Re_v6_C2_v55a	-502.01972226	39.99	
113	2-PressCapCube_Re_v4_C2_v44c	-502.01953831	40.11	
114	2-PressCapCube_Re_v4_C2_v54a	-502.01926828	40.27	C-C
115	4-TrTrPr_Re_v5_C2_v54d_r-122	-502.01926204	40.28	
116	3-Tl99-Re_v5a_C2_v44d	-502.01926203	40.28	
117	3-Tl99-Re_v5b_C2_v44d_r-228	-502.01910659	40.38	C-C
118	3-Tl99-Re_v5b_C2_v64b	-502.01910659	40.38	C-C
119	3-Tl99-Re_v4_C2-b	-502.01598150	42.34	
120	3-Tl99-Re_v5b_C2_v64a	-502.01542332	42.69	C-C
121	4-TrTrPr_Re_v5_C2_v54e	-502.01542332	42.69	C-C
122	3-Tl99-Re_v5b_C2_v54b	-502.01542331	42.69	C-C
123	3-Tl99-Re_v5a_C2_v64a	-502.01489503	43.02	C-C
124	4-TrTrPr_Re_v5_C2_v55b	-502.01489503	43.02	C-C
125	3-Tl99-Re_v4_C2-k	-502.01489502	43.02	C-C
126	3-Tl99-Re_v5b_C2_v55b	-502.01489502	43.02	C-C
127	2-PressCapCube_Re_v4_C2_v54c	-502.01406413	43.54	C-C
128	3-Tl99-Re_v5b_C2_v55a	-502.01406413	43.54	C-C
129	4-TrTrPr_Re_v5_C2_v54b	-502.01406413	43.54	C-C
130	4-TrTrPr_Re_v5_C2_v45 imag	-502.01397279	43.60	
131	4-TrTrPr_Re_v5_C2_v55a	-502.01339305	43.96	
132	3-Tl99-Re_v4_C2-l	-502.01339303	43.96	
133	4-TrTrPr_Re_v5_C2_v44b i-58	-502.01335663	43.98	
134	1-CapCube_Re_v4b_C2_v44e	-502.01268364	44.41	C-C
135	1-CapCube_Re_v4b_C2_v44d	-502.01241895	44.57	C-C
136	2-PressCapCube_Re_v5_C2_v44e	-502.01010525	46.02	
137	3-Tl99-Re_v5b_C2_v45a	-502.00957944	46.35	C-C
138	4-TrTrPr_Re_v5_C2_v54a	-502.00957944	46.35	C-C
139	3-Tl99-Re_v4_C2-c	-502.00845785	47.06	C-C
140	1-CapCube_Re_v4b_C2_v43e	-502.00842410	47.08	C-C
141	4-TrTrPr_Re_v4_C2_v44	-502.00823295	47.20	
142	3-Tl99-Re_v4_C2-u	-502.00788806	47.42	C-C
143	2-PressCapCube_Re_v4_C2_v53	-502.00757247	47.61	
144	4-TrTrPr_Re_v4_C2_v54b	-502.00628805	48.42	C-C
145	3-Tl99-Re_v5b_C2_v44d i-228	-502.00403470	49.83	C-C
146	3-Tl99-Re_v5a_C2_v65b	-502.00080308	51.86	

147	3-Tl99-Re_v5a_C2_v54b	-502.00000924	52.36	C-C
148	4-TrTrPr_Re_v5_C2_v54d i-122	-501.99625148	54.72	
149	3-Tl99-Re_v4_C2-z	-501.99355351	56.41	C-C
150	3-Tl99-Re_v5b_C2_v44a_r-50	-501.98953385	58.93	C-C
151	4-TrTrPr_Re_v4_C2_v55d_r-50	-501.98953385	58.93	C-C
152	3-Tl99-Re_v5a_C2_v44a	-501.98833664	59.68	C-C
153	3-Tl99-Re_v4_C2-a	-501.98826906	59.73	C-C
154	3-Tl99-Re_v5b_C2_v44a i-50	-501.98795125	59.93	C-C
155	4-TrTrPr_Re_v4_C2_v55d i-50	-501.98795125	59.93	C-C
156	3-Tl99-Re_v5a_C2_v55b	-501.98734308	60.31	C-C
157	3-Tl99-Re_v4_C2-f	-501.98615654	61.05	
158	2- PressCapCube_Re_v4_C2_v43b	-501.98474411	61.94	C-C
159	4-TrTrPr_Re_v4_C2_v55a_r-58	-501.98470634	61.96	C-C
160	4-TrTrPr_Re_v4_C2_v55a i-58	-501.98223914	63.51	C-C
161	1-CapCube_Re_v4_C2_v33b	-501.98159486	63.91	C-C
162	3-Tl99-Re_v5a_C2_v64b	-501.98018400	64.80	C-C
163	3-Tl99-Re_v5a_C2_v54c	-501.97916919	65.44	C-C
164	1-CapCube_Re_v4b_C2_v33a	-501.97916918	65.44	C-C
165	3-Tl99-Re_v4_C2-w	-501.97651546	67.10	C-C
166	3-Tl99-Re_v4_C2-t	-501.97551772	67.73	C-C
167	2- PressCapCube_Re_v4_C2_v43a	-501.97402322	68.67	C-C
168	3-Tl99-Re_v4_C2-x	-501.97227110	69.77	C-C
169	3-Tl99-Re_v4_C2-zz	-501.97227109	69.77	C-C
170	3-Tl99-Re_v4_C2-j	-501.96704382	73.05	C-C
171	3-Tl99-Re_v4_C2-d	-501.96124212	76.69	C-C
172	2- PressCapCube_Re_v4_C2_v44a	-501.96075987	76.99	C-C
173	3-Tl99-Re_v4_C2-i	-501.95830611	78.53	
174	3-Tl99-Re_v4_C2-y	-501.95648901	79.67	
175	3-Tl99-Re_v4_C2-z	-501.93761943	91.51	C-C

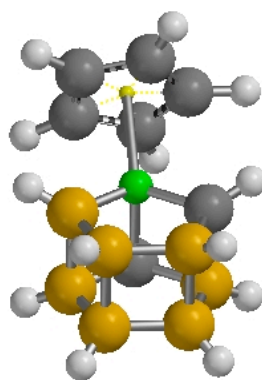
10-vertex $\text{CpMnC}_2\text{B}_7\text{H}_9$

Table 1. Initial structures (one example from each family) 316 structures in total

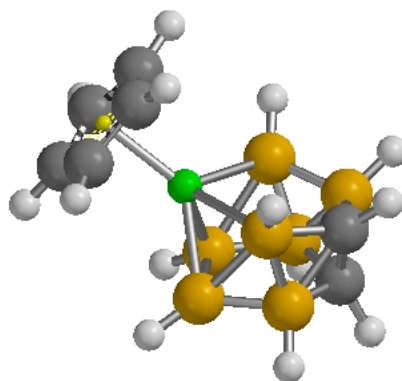
Initial structures
 <p>1. Tetracapped trigonal prism 41 structures</p>
 <p>2. Tetracapped trigonal prism 84 structures</p>
 <p>3. Bicapped cube 33 structures</p>



4. Bicapped square antiprism 34 structures



5. Pentacapped prism 20 structures



6. Antiprism 20 structures

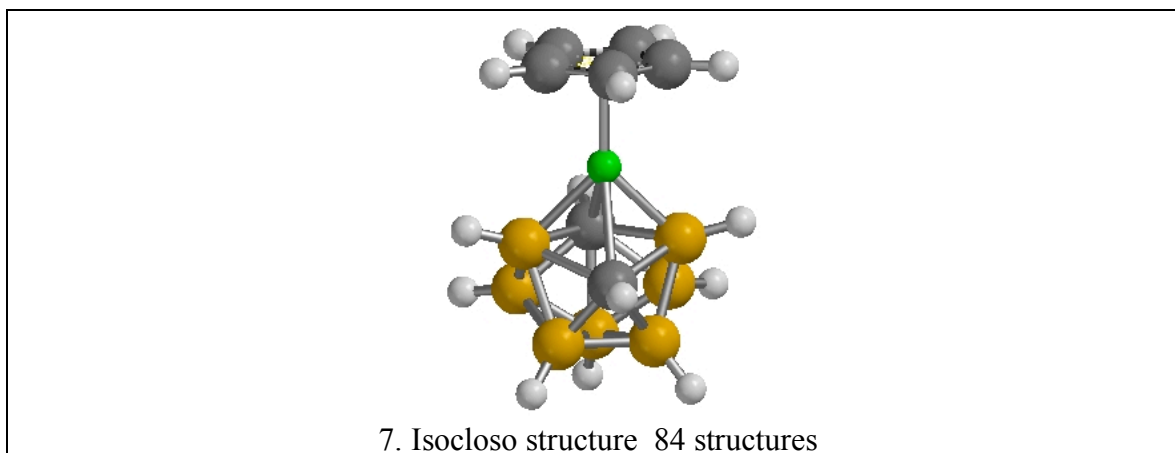
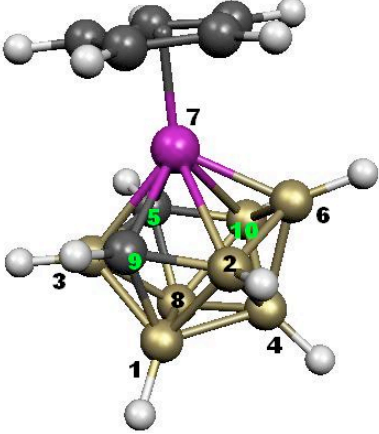
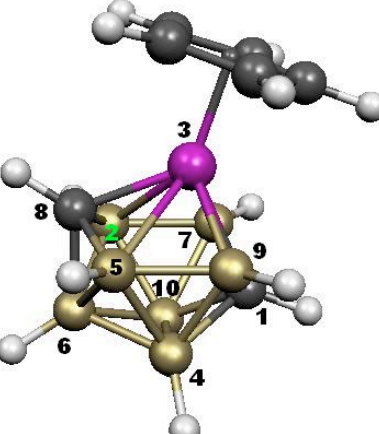
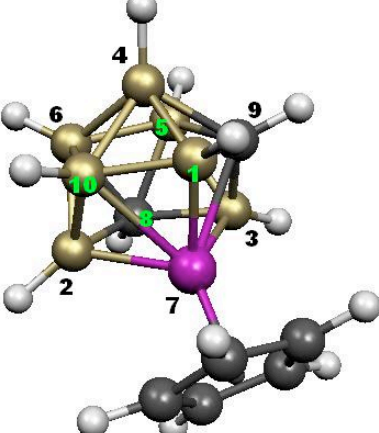
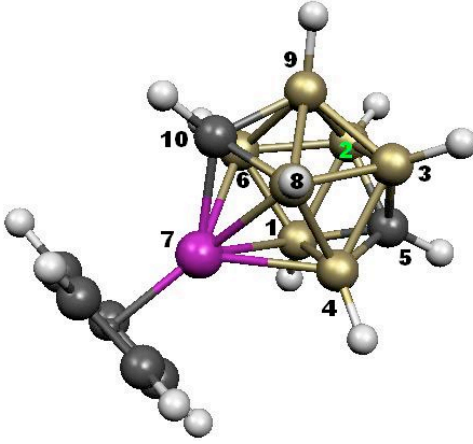
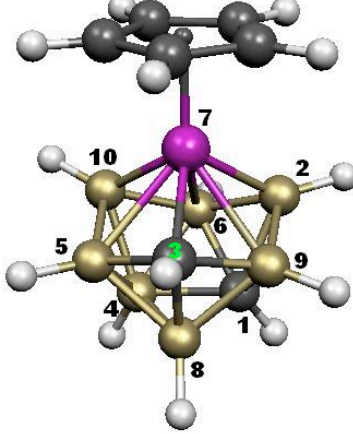
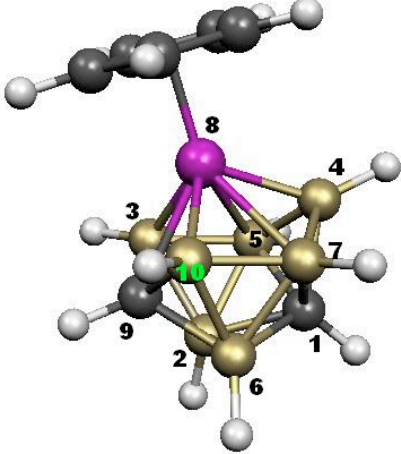
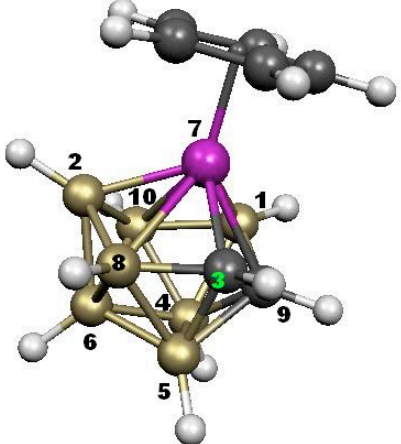
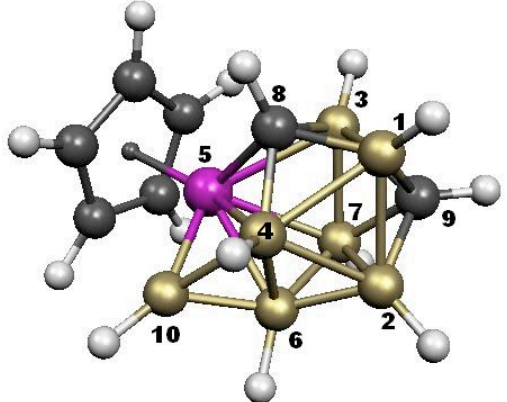
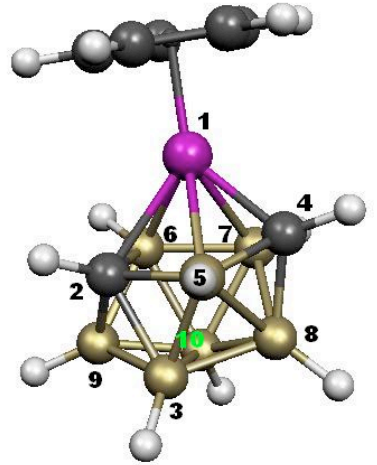
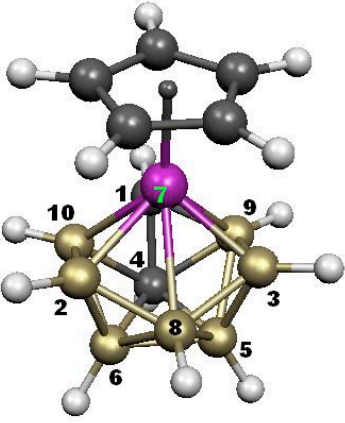
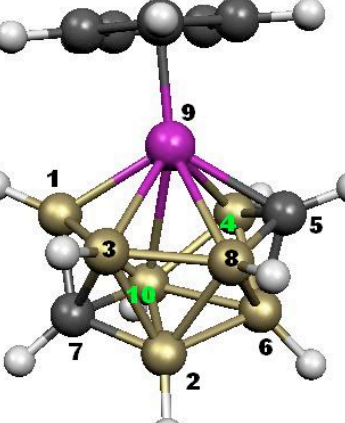
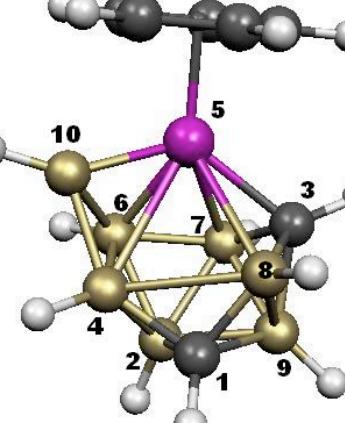


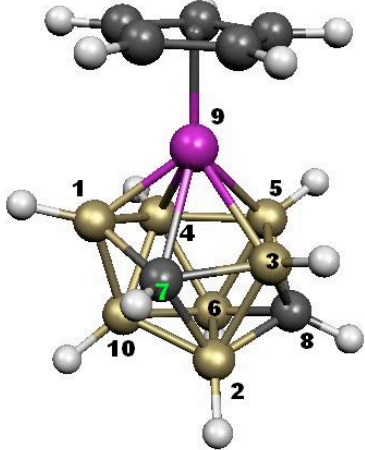
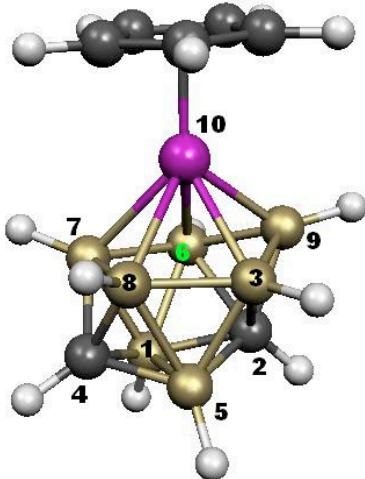
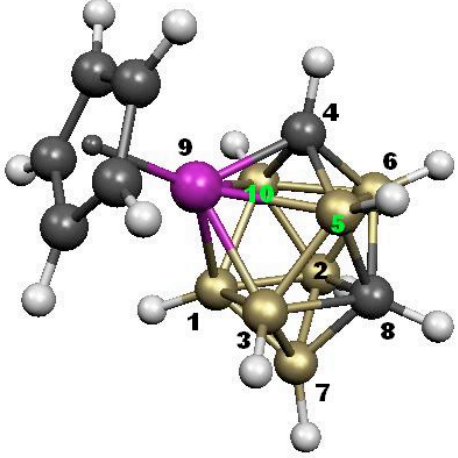
Table 2. Distance table for the best structures

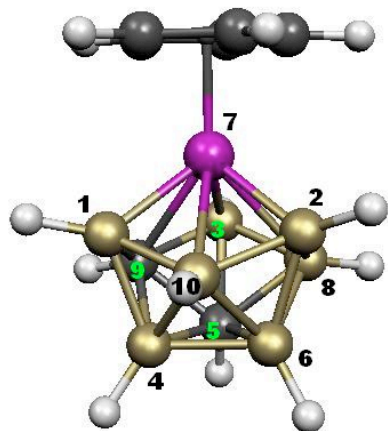
 <p>1. -1600.14169157 Cs 0.0 kcal/mole</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.801537</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.856913</td><td>2.739835</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.796510</td><td>1.810504</td><td>2.881625</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>2.745681</td><td>3.153157</td><td>1.610045</td><td>2.719140</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.938595</td><td>1.760861</td><td>3.310562</td><td>1.810931</td><td>2.785035</td></tr> <tr><td>7 Mn</td><td>2.964719</td><td>2.263888</td><td>2.231017</td><td>2.923983</td><td>1.945860</td></tr> <tr><td>8 B</td><td>1.797565</td><td>2.873675</td><td>1.856891</td><td>1.796696</td><td>1.658969</td></tr> <tr><td>9 C</td><td>1.659364</td><td>1.587368</td><td>1.609615</td><td>2.719536</td><td>2.662603</td></tr> <tr><td>10 B</td><td>2.873683</td><td>2.787909</td><td>2.740273</td><td>1.810328</td><td>1.587344</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 Mn</td><td>1.970614</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.938963</td><td>2.964392</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>2.784972</td><td>1.946517</td><td>2.745780</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.760854</td><td>2.263045</td><td>1.802118</td><td>3.153282</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.801537	0.000000				3 B	1.856913	2.739835	0.000000			4 B	1.796510	1.810504	2.881625	0.000000		5 C	2.745681	3.153157	1.610045	2.719140	0.000000	6 B	2.938595	1.760861	3.310562	1.810931	2.785035	7 Mn	2.964719	2.263888	2.231017	2.923983	1.945860	8 B	1.797565	2.873675	1.856891	1.796696	1.658969	9 C	1.659364	1.587368	1.609615	2.719536	2.662603	10 B	2.873683	2.787909	2.740273	1.810328	1.587344		6	7	8	9	10	6 B	0.000000					7 Mn	1.970614	0.000000				8 B	2.938963	2.964392	0.000000			9 C	2.784972	1.946517	2.745780	0.000000		10 B	1.760854	2.263045	1.802118	3.153282	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.801537	0.000000																																																																																																					
3 B	1.856913	2.739835	0.000000																																																																																																				
4 B	1.796510	1.810504	2.881625	0.000000																																																																																																			
5 C	2.745681	3.153157	1.610045	2.719140	0.000000																																																																																																		
6 B	2.938595	1.760861	3.310562	1.810931	2.785035																																																																																																		
7 Mn	2.964719	2.263888	2.231017	2.923983	1.945860																																																																																																		
8 B	1.797565	2.873675	1.856891	1.796696	1.658969																																																																																																		
9 C	1.659364	1.587368	1.609615	2.719536	2.662603																																																																																																		
10 B	2.873683	2.787909	2.740273	1.810328	1.587344																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Mn	1.970614	0.000000																																																																																																					
8 B	2.938963	2.964392	0.000000																																																																																																				
9 C	2.784972	1.946517	2.745780	0.000000																																																																																																			
10 B	1.760854	2.263045	1.802118	3.153282	0.000000																																																																																																		
 <p>2. -1600.13831317 Cs +2.1</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.641583</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Mn</td><td>2.189796</td><td>2.258288</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.709799</td><td>2.865482</td><td>2.936838</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.642460</td><td>2.759350</td><td>2.257894</td><td>1.811962</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.738605</td><td>1.832917</td><td>2.968741</td><td>1.786060</td><td>1.833225</td></tr> <tr><td>7 B</td><td>1.638403</td><td>1.743853</td><td>1.975722</td><td>2.879771</td><td>3.297552</td></tr> <tr><td>8 C</td><td>3.003100</td><td>1.603931</td><td>1.942777</td><td>2.700564</td><td>1.603579</td></tr> <tr><td>9 B</td><td>1.637745</td><td>3.296195</td><td>1.975609</td><td>1.793059</td><td>1.743508</td></tr> <tr><td>10 B</td><td>1.708479</td><td>1.811428</td><td>2.936327</td><td>1.785895</td><td>2.865189</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.922793</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>1.644758</td><td>2.775672</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.921260</td><td>2.837246</td><td>2.774953</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.785848</td><td>1.794748</td><td>2.700242</td><td>2.877003</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	2.641583	0.000000				3 Mn	2.189796	2.258288	0.000000			4 B	1.709799	2.865482	2.936838	0.000000		5 B	2.642460	2.759350	2.257894	1.811962	0.000000	6 B	2.738605	1.832917	2.968741	1.786060	1.833225	7 B	1.638403	1.743853	1.975722	2.879771	3.297552	8 C	3.003100	1.603931	1.942777	2.700564	1.603579	9 B	1.637745	3.296195	1.975609	1.793059	1.743508	10 B	1.708479	1.811428	2.936327	1.785895	2.865189		6	7	8	9	10	6 B	0.000000					7 B	2.922793	0.000000				8 C	1.644758	2.775672	0.000000			9 B	2.921260	2.837246	2.774953	0.000000		10 B	1.785848	1.794748	2.700242	2.877003	0.000000
	1	2	3	4	5																																																																																																		
1 C	0.000000																																																																																																						
2 B	2.641583	0.000000																																																																																																					
3 Mn	2.189796	2.258288	0.000000																																																																																																				
4 B	1.709799	2.865482	2.936838	0.000000																																																																																																			
5 B	2.642460	2.759350	2.257894	1.811962	0.000000																																																																																																		
6 B	2.738605	1.832917	2.968741	1.786060	1.833225																																																																																																		
7 B	1.638403	1.743853	1.975722	2.879771	3.297552																																																																																																		
8 C	3.003100	1.603931	1.942777	2.700564	1.603579																																																																																																		
9 B	1.637745	3.296195	1.975609	1.793059	1.743508																																																																																																		
10 B	1.708479	1.811428	2.936327	1.785895	2.865189																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	2.922793	0.000000																																																																																																					
8 C	1.644758	2.775672	0.000000																																																																																																				
9 B	2.921260	2.837246	2.774953	0.000000																																																																																																			
10 B	1.785848	1.794748	2.700242	2.877003	0.000000																																																																																																		
 <p>3. -1600.12510354 Cs +10.4</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>2.865869</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.833110</td><td>2.833231</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.771127</td><td>2.870490</td><td>2.882262</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.842002</td><td>2.842304</td><td>1.797694</td><td>1.767676</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.869884</td><td>1.771292</td><td>2.882336</td><td>1.779841</td><td>1.767877</td></tr> <tr><td>7 Mn</td><td>1.988270</td><td>1.988586</td><td>1.956635</td><td>2.960674</td><td>2.941376</td></tr> <tr><td>8 C</td><td>3.143715</td><td>1.647743</td><td>1.634265</td><td>2.733295</td><td>1.704551</td></tr> <tr><td>9 C</td><td>1.647729</td><td>3.144016</td><td>1.634241</td><td>1.737342</td><td>1.704457</td></tr> <tr><td>10 B</td><td>1.724538</td><td>1.724682</td><td>3.288943</td><td>1.797354</td><td>2.838970</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 Mn</td><td>2.960641</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>1.737465</td><td>2.189111</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>2.733247</td><td>2.188957</td><td>2.501459</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.796907</td><td>2.304436</td><td>2.659271</td><td>2.659420</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.865869	0.000000				3 B	2.833110	2.833231	0.000000			4 B	1.771127	2.870490	2.882262	0.000000		5 B	2.842002	2.842304	1.797694	1.767676	0.000000	6 B	2.869884	1.771292	2.882336	1.779841	1.767877	7 Mn	1.988270	1.988586	1.956635	2.960674	2.941376	8 C	3.143715	1.647743	1.634265	2.733295	1.704551	9 C	1.647729	3.144016	1.634241	1.737342	1.704457	10 B	1.724538	1.724682	3.288943	1.797354	2.838970		6	7	8	9	10	6 B	0.000000					7 Mn	2.960641	0.000000				8 C	1.737465	2.189111	0.000000			9 C	2.733247	2.188957	2.501459	0.000000		10 B	1.796907	2.304436	2.659271	2.659420	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	2.865869	0.000000																																																																																																					
3 B	2.833110	2.833231	0.000000																																																																																																				
4 B	1.771127	2.870490	2.882262	0.000000																																																																																																			
5 B	2.842002	2.842304	1.797694	1.767676	0.000000																																																																																																		
6 B	2.869884	1.771292	2.882336	1.779841	1.767877																																																																																																		
7 Mn	1.988270	1.988586	1.956635	2.960674	2.941376																																																																																																		
8 C	3.143715	1.647743	1.634265	2.733295	1.704551																																																																																																		
9 C	1.647729	3.144016	1.634241	1.737342	1.704457																																																																																																		
10 B	1.724538	1.724682	3.288943	1.797354	2.838970																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Mn	2.960641	0.000000																																																																																																					
8 C	1.737465	2.189111	0.000000																																																																																																				
9 C	2.733247	2.188957	2.501459	0.000000																																																																																																			
10 B	1.796907	2.304436	2.659271	2.659420	0.000000																																																																																																		

 <p>4. -1600.12070009 Cs +13.2</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.860954</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.621153</td><td>1.829400</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.862500</td><td>2.621100</td><td>1.860899</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>1.592939</td><td>1.606811</td><td>1.606825</td><td>1.592960</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.814253</td><td>1.834715</td><td>2.856212</td><td>2.858248</td><td>2.767777</td></tr> <tr><td>7 Mn</td><td>2.191606</td><td>3.341569</td><td>3.341532</td><td>2.191489</td><td>3.221884</td></tr> <tr><td>8 B</td><td>2.858283</td><td>2.856164</td><td>1.834650</td><td>1.814099</td><td>2.767722</td></tr> <tr><td>9 B</td><td>2.859581</td><td>1.784835</td><td>1.784790</td><td>2.859458</td><td>2.751832</td></tr> <tr><td>10 C</td><td>2.832632</td><td>2.777563</td><td>2.777549</td><td>2.832517</td><td>3.397823</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 Mn</td><td>2.167861</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.619300</td><td>2.167788</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.881086</td><td>3.069968</td><td>1.881012</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>1.625333</td><td>1.909689</td><td>1.625332</td><td>1.607369</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.860954	0.000000				3 B	2.621153	1.829400	0.000000			4 B	1.862500	2.621100	1.860899	0.000000		5 C	1.592939	1.606811	1.606825	1.592960	0.000000	6 B	1.814253	1.834715	2.856212	2.858248	2.767777	7 Mn	2.191606	3.341569	3.341532	2.191489	3.221884	8 B	2.858283	2.856164	1.834650	1.814099	2.767722	9 B	2.859581	1.784835	1.784790	2.859458	2.751832	10 C	2.832632	2.777563	2.777549	2.832517	3.397823		6	7	8	9	10	6 B	0.000000					7 Mn	2.167861	0.000000				8 B	2.619300	2.167788	0.000000			9 B	1.881086	3.069968	1.881012	0.000000		10 C	1.625333	1.909689	1.625332	1.607369	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.860954	0.000000																																																																																																					
3 B	2.621153	1.829400	0.000000																																																																																																				
4 B	1.862500	2.621100	1.860899	0.000000																																																																																																			
5 C	1.592939	1.606811	1.606825	1.592960	0.000000																																																																																																		
6 B	1.814253	1.834715	2.856212	2.858248	2.767777																																																																																																		
7 Mn	2.191606	3.341569	3.341532	2.191489	3.221884																																																																																																		
8 B	2.858283	2.856164	1.834650	1.814099	2.767722																																																																																																		
9 B	2.859581	1.784835	1.784790	2.859458	2.751832																																																																																																		
10 C	2.832632	2.777563	2.777549	2.832517	3.397823																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Mn	2.167861	0.000000																																																																																																					
8 B	2.619300	2.167788	0.000000																																																																																																				
9 B	1.881086	3.069968	1.881012	0.000000																																																																																																			
10 C	1.625333	1.909689	1.625332	1.607369	0.000000																																																																																																		
 <p>5. -1600.11976890 +13.8</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.730968</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.596704</td><td>2.790093</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.717257</td><td>2.892039</td><td>2.728503</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.731688</td><td>3.301246</td><td>1.595338</td><td>1.821751</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.699093</td><td>1.717964</td><td>3.162154</td><td>1.768872</td><td>2.767158</td></tr> <tr><td>7 Mn</td><td>2.797996</td><td>1.973532</td><td>1.956207</td><td>2.939625</td><td>2.265214</td></tr> <tr><td>8 B</td><td>1.706159</td><td>2.911828</td><td>1.648215</td><td>1.792307</td><td>1.806726</td></tr> <tr><td>9 B</td><td>1.742634</td><td>1.734473</td><td>1.588061</td><td>2.867782</td><td>2.722584</td></tr> <tr><td>10 B</td><td>2.770501</td><td>2.871462</td><td>2.792877</td><td>1.790465</td><td>1.752935</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 Mn</td><td>2.296197</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.843586</td><td>2.955896</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.754993</td><td>2.228773</td><td>1.820679</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.719453</td><td>1.989791</td><td>2.912347</td><td>3.289043</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.730968	0.000000				3 C	2.596704	2.790093	0.000000			4 B	1.717257	2.892039	2.728503	0.000000		5 B	2.731688	3.301246	1.595338	1.821751	0.000000	6 B	1.699093	1.717964	3.162154	1.768872	2.767158	7 Mn	2.797996	1.973532	1.956207	2.939625	2.265214	8 B	1.706159	2.911828	1.648215	1.792307	1.806726	9 B	1.742634	1.734473	1.588061	2.867782	2.722584	10 B	2.770501	2.871462	2.792877	1.790465	1.752935		6	7	8	9	10	6 B	0.000000					7 Mn	2.296197	0.000000				8 B	2.843586	2.955896	0.000000			9 B	2.754993	2.228773	1.820679	0.000000		10 B	1.719453	1.989791	2.912347	3.289043	0.000000
	1	2	3	4	5																																																																																																		
1 C	0.000000																																																																																																						
2 B	1.730968	0.000000																																																																																																					
3 C	2.596704	2.790093	0.000000																																																																																																				
4 B	1.717257	2.892039	2.728503	0.000000																																																																																																			
5 B	2.731688	3.301246	1.595338	1.821751	0.000000																																																																																																		
6 B	1.699093	1.717964	3.162154	1.768872	2.767158																																																																																																		
7 Mn	2.797996	1.973532	1.956207	2.939625	2.265214																																																																																																		
8 B	1.706159	2.911828	1.648215	1.792307	1.806726																																																																																																		
9 B	1.742634	1.734473	1.588061	2.867782	2.722584																																																																																																		
10 B	2.770501	2.871462	2.792877	1.790465	1.752935																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Mn	2.296197	0.000000																																																																																																					
8 B	2.843586	2.955896	0.000000																																																																																																				
9 B	2.754993	2.228773	1.820679	0.000000																																																																																																			
10 B	1.719453	1.989791	2.912347	3.289043	0.000000																																																																																																		
 <p>6. -1600.11030842 Cs +19.7</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.699921</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.766010</td><td>1.769543</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.710524</td><td>2.856378</td><td>2.875636</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.733161</td><td>1.766535</td><td>1.714403</td><td>1.727784</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.700342</td><td>1.800259</td><td>2.873340</td><td>2.856548</td><td>2.852086</td></tr> <tr><td>7 B</td><td>1.733060</td><td>2.851800</td><td>3.296512</td><td>1.727583</td><td>2.784486</td></tr> <tr><td>8 Mn</td><td>2.811727</td><td>2.936944</td><td>1.990115</td><td>1.974247</td><td>2.280325</td></tr> <tr><td>9 C</td><td>2.593320</td><td>1.710571</td><td>1.642542</td><td>3.150552</td><td>2.629551</td></tr> <tr><td>10 B</td><td>2.766381</td><td>2.873839</td><td>2.847288</td><td>2.875593</td><td>3.296746</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.766612</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Mn</td><td>2.936912</td><td>2.280476</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.710221</td><td>2.629496</td><td>2.203220</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.769757</td><td>1.714608</td><td>1.990057</td><td>1.642792</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.699921	0.000000				3 B	2.766010	1.769543	0.000000			4 B	1.710524	2.856378	2.875636	0.000000		5 B	1.733161	1.766535	1.714403	1.727784	0.000000	6 B	1.700342	1.800259	2.873340	2.856548	2.852086	7 B	1.733060	2.851800	3.296512	1.727583	2.784486	8 Mn	2.811727	2.936944	1.990115	1.974247	2.280325	9 C	2.593320	1.710571	1.642542	3.150552	2.629551	10 B	2.766381	2.873839	2.847288	2.875593	3.296746		6	7	8	9	10	6 B	0.000000					7 B	1.766612	0.000000				8 Mn	2.936912	2.280476	0.000000			9 C	1.710221	2.629496	2.203220	0.000000		10 B	1.769757	1.714608	1.990057	1.642792	0.000000
	1	2	3	4	5																																																																																																		
1 C	0.000000																																																																																																						
2 B	1.699921	0.000000																																																																																																					
3 B	2.766010	1.769543	0.000000																																																																																																				
4 B	1.710524	2.856378	2.875636	0.000000																																																																																																			
5 B	1.733161	1.766535	1.714403	1.727784	0.000000																																																																																																		
6 B	1.700342	1.800259	2.873340	2.856548	2.852086																																																																																																		
7 B	1.733060	2.851800	3.296512	1.727583	2.784486																																																																																																		
8 Mn	2.811727	2.936944	1.990115	1.974247	2.280325																																																																																																		
9 C	2.593320	1.710571	1.642542	3.150552	2.629551																																																																																																		
10 B	2.766381	2.873839	2.847288	2.875593	3.296746																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	1.766612	0.000000																																																																																																					
8 Mn	2.936912	2.280476	0.000000																																																																																																				
9 C	1.710221	2.629496	2.203220	0.000000																																																																																																			
10 B	1.769757	1.714608	1.990057	1.642792	0.000000																																																																																																		

 <p>7. -1600.10947096 +20.2</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>2.859568</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.750663</td><td>2.779848</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.789974</td><td>2.875247</td><td>2.721736</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.904654</td><td>2.906496</td><td>1.677698</td><td>1.786822</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.891425</td><td>1.785467</td><td>2.729112</td><td>1.789817</td><td>1.780065</td></tr> <tr><td>7 Mn</td><td>1.989841</td><td>1.995830</td><td>1.925684</td><td>2.955547</td><td>2.976036</td></tr> <tr><td>8 B</td><td>3.283929</td><td>1.755321</td><td>1.590173</td><td>2.863083</td><td>1.812228</td></tr> <tr><td>9 C</td><td>1.655522</td><td>3.155882</td><td>1.527808</td><td>1.745418</td><td>1.759334</td></tr> <tr><td>10 B</td><td>1.710320</td><td>1.730084</td><td>3.162072</td><td>1.767932</td><td>2.860793</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 Mn</td><td>2.957440</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.829411</td><td>2.251940</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>2.745875</td><td>2.162010</td><td>2.611586</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.800606</td><td>2.326004</td><td>2.792800</td><td>2.641103</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.859568	0.000000				3 C	2.750663	2.779848	0.000000			4 B	1.789974	2.875247	2.721736	0.000000		5 B	2.904654	2.906496	1.677698	1.786822	0.000000	6 B	2.891425	1.785467	2.729112	1.789817	1.780065	7 Mn	1.989841	1.995830	1.925684	2.955547	2.976036	8 B	3.283929	1.755321	1.590173	2.863083	1.812228	9 C	1.655522	3.155882	1.527808	1.745418	1.759334	10 B	1.710320	1.730084	3.162072	1.767932	2.860793		6	7	8	9	10	6 B	0.000000					7 Mn	2.957440	0.000000				8 B	1.829411	2.251940	0.000000			9 C	2.745875	2.162010	2.611586	0.000000		10 B	1.800606	2.326004	2.792800	2.641103	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	2.859568	0.000000																																																																																																					
3 C	2.750663	2.779848	0.000000																																																																																																				
4 B	1.789974	2.875247	2.721736	0.000000																																																																																																			
5 B	2.904654	2.906496	1.677698	1.786822	0.000000																																																																																																		
6 B	2.891425	1.785467	2.729112	1.789817	1.780065																																																																																																		
7 Mn	1.989841	1.995830	1.925684	2.955547	2.976036																																																																																																		
8 B	3.283929	1.755321	1.590173	2.863083	1.812228																																																																																																		
9 C	1.655522	3.155882	1.527808	1.745418	1.759334																																																																																																		
10 B	1.710320	1.730084	3.162072	1.767932	2.860793																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Mn	2.957440	0.000000																																																																																																					
8 B	1.829411	2.251940	0.000000																																																																																																				
9 C	2.745875	2.162010	2.611586	0.000000																																																																																																			
10 B	1.800606	2.326004	2.792800	2.641103	0.000000																																																																																																		
 <p>8. -1600.10092144 +25.6</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.990114</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.819001</td><td>2.655387</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.043214</td><td>2.011511</td><td>2.688042</td><td>0.000000</td><td></td></tr> <tr><td>5 Mn</td><td>3.132371</td><td>3.132354</td><td>2.206624</td><td>2.207228</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.983671</td><td>1.683728</td><td>2.923503</td><td>1.799866</td><td>2.111626</td></tr> <tr><td>7 B</td><td>2.680969</td><td>1.870538</td><td>1.868170</td><td>2.723537</td><td>2.230538</td></tr> <tr><td>8 C</td><td>1.593518</td><td>2.758284</td><td>1.640049</td><td>1.619118</td><td>1.974929</td></tr> <tr><td>9 C</td><td>1.580004</td><td>1.590507</td><td>1.630950</td><td>2.790208</td><td>3.185906</td></tr> <tr><td>10 B</td><td>3.828705</td><td>3.160084</td><td>3.662604</td><td>1.989641</td><td>1.852165</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.742634</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.798413</td><td>2.762709</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>2.688952</td><td>1.640459</td><td>2.546447</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.681386</td><td>3.054195</td><td>2.952638</td><td>4.025469</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.990114	0.000000				3 B	1.819001	2.655387	0.000000			4 B	2.043214	2.011511	2.688042	0.000000		5 Mn	3.132371	3.132354	2.206624	2.207228	0.000000	6 B	2.983671	1.683728	2.923503	1.799866	2.111626	7 B	2.680969	1.870538	1.868170	2.723537	2.230538	8 C	1.593518	2.758284	1.640049	1.619118	1.974929	9 C	1.580004	1.590507	1.630950	2.790208	3.185906	10 B	3.828705	3.160084	3.662604	1.989641	1.852165		6	7	8	9	10	6 B	0.000000					7 B	1.742634	0.000000				8 C	2.798413	2.762709	0.000000			9 C	2.688952	1.640459	2.546447	0.000000		10 B	1.681386	3.054195	2.952638	4.025469	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.990114	0.000000																																																																																																					
3 B	1.819001	2.655387	0.000000																																																																																																				
4 B	2.043214	2.011511	2.688042	0.000000																																																																																																			
5 Mn	3.132371	3.132354	2.206624	2.207228	0.000000																																																																																																		
6 B	2.983671	1.683728	2.923503	1.799866	2.111626																																																																																																		
7 B	2.680969	1.870538	1.868170	2.723537	2.230538																																																																																																		
8 C	1.593518	2.758284	1.640049	1.619118	1.974929																																																																																																		
9 C	1.580004	1.590507	1.630950	2.790208	3.185906																																																																																																		
10 B	3.828705	3.160084	3.662604	1.989641	1.852165																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	1.742634	0.000000																																																																																																					
8 C	2.798413	2.762709	0.000000																																																																																																				
9 C	2.688952	1.640459	2.546447	0.000000																																																																																																			
10 B	1.681386	3.054195	2.952638	4.025469	0.000000																																																																																																		
 <p>9. -1600.09809624 +27.6</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 Mn</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 C</td><td>2.178253</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.357853</td><td>1.759389</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.905519</td><td>2.718643</td><td>2.776433</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.188012</td><td>1.691510</td><td>1.808815</td><td>1.627035</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.082026</td><td>1.737414</td><td>2.596755</td><td>2.765761</td><td>2.749613</td></tr> <tr><td>7 B</td><td>2.148189</td><td>2.744575</td><td>2.846402</td><td>1.623705</td><td>2.597702</td></tr> <tr><td>8 B</td><td>3.067543</td><td>2.714044</td><td>1.771992</td><td>1.615638</td><td>1.872758</td></tr> <tr><td>9 B</td><td>3.354800</td><td>1.625744</td><td>1.716567</td><td>3.566641</td><td>2.873457</td></tr> <tr><td>10 B</td><td>3.337229</td><td>2.483491</td><td>1.811790</td><td>2.806269</td><td>2.832156</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.799818</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.817364</td><td>1.860500</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.711020</td><td>2.923659</td><td>2.898546</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.880587</td><td>1.856168</td><td>1.797510</td><td>1.693196</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 Mn	0.000000					2 C	2.178253	0.000000				3 B	3.357853	1.759389	0.000000			4 C	1.905519	2.718643	2.776433	0.000000		5 B	2.188012	1.691510	1.808815	1.627035	0.000000	6 B	2.082026	1.737414	2.596755	2.765761	2.749613	7 B	2.148189	2.744575	2.846402	1.623705	2.597702	8 B	3.067543	2.714044	1.771992	1.615638	1.872758	9 B	3.354800	1.625744	1.716567	3.566641	2.873457	10 B	3.337229	2.483491	1.811790	2.806269	2.832156		6	7	8	9	10	6 B	0.000000					7 B	1.799818	0.000000				8 B	2.817364	1.860500	0.000000			9 B	1.711020	2.923659	2.898546	0.000000		10 B	1.880587	1.856168	1.797510	1.693196	0.000000
	1	2	3	4	5																																																																																																		
1 Mn	0.000000																																																																																																						
2 C	2.178253	0.000000																																																																																																					
3 B	3.357853	1.759389	0.000000																																																																																																				
4 C	1.905519	2.718643	2.776433	0.000000																																																																																																			
5 B	2.188012	1.691510	1.808815	1.627035	0.000000																																																																																																		
6 B	2.082026	1.737414	2.596755	2.765761	2.749613																																																																																																		
7 B	2.148189	2.744575	2.846402	1.623705	2.597702																																																																																																		
8 B	3.067543	2.714044	1.771992	1.615638	1.872758																																																																																																		
9 B	3.354800	1.625744	1.716567	3.566641	2.873457																																																																																																		
10 B	3.337229	2.483491	1.811790	2.806269	2.832156																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	1.799818	0.000000																																																																																																					
8 B	2.817364	1.860500	0.000000																																																																																																				
9 B	1.711020	2.923659	2.898546	0.000000																																																																																																			
10 B	1.880587	1.856168	1.797510	1.693196	0.000000																																																																																																		

 <p>10. -1600.09771710 Cs +27.6</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.783848</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.783893</td><td>2.878801</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.593051</td><td>2.786079</td><td>2.786109</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.722198</td><td>2.896299</td><td>1.786592</td><td>1.702895</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.722161</td><td>1.786518</td><td>2.896413</td><td>1.702902</td><td>1.805300</td></tr> <tr><td>7 Mn</td><td>1.923493</td><td>2.001350</td><td>2.001229</td><td>2.820340</td><td>2.945543</td></tr> <tr><td>8 B</td><td>3.159249</td><td>1.724131</td><td>1.724138</td><td>2.712458</td><td>1.774063</td></tr> <tr><td>9 B</td><td>1.604046</td><td>3.309780</td><td>1.738892</td><td>1.753010</td><td>1.822171</td></tr> <tr><td>10 B</td><td>1.604024</td><td>1.738902</td><td>3.309845</td><td>1.753020</td><td>2.879880</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 Mn</td><td>2.945598</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.774149</td><td>2.325893</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.879904</td><td>2.248453</td><td>2.771600</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.822097</td><td>2.248600</td><td>2.771643</td><td>2.755001</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	2.783848	0.000000				3 B	2.783893	2.878801	0.000000			4 C	1.593051	2.786079	2.786109	0.000000		5 B	2.722198	2.896299	1.786592	1.702895	0.000000	6 B	2.722161	1.786518	2.896413	1.702902	1.805300	7 Mn	1.923493	2.001350	2.001229	2.820340	2.945543	8 B	3.159249	1.724131	1.724138	2.712458	1.774063	9 B	1.604046	3.309780	1.738892	1.753010	1.822171	10 B	1.604024	1.738902	3.309845	1.753020	2.879880		6	7	8	9	10	6 B	0.000000					7 Mn	2.945598	0.000000				8 B	1.774149	2.325893	0.000000			9 B	2.879904	2.248453	2.771600	0.000000		10 B	1.822097	2.248600	2.771643	2.755001	0.000000
	1	2	3	4	5																																																																																																		
1 C	0.000000																																																																																																						
2 B	2.783848	0.000000																																																																																																					
3 B	2.783893	2.878801	0.000000																																																																																																				
4 C	1.593051	2.786079	2.786109	0.000000																																																																																																			
5 B	2.722198	2.896299	1.786592	1.702895	0.000000																																																																																																		
6 B	2.722161	1.786518	2.896413	1.702902	1.805300																																																																																																		
7 Mn	1.923493	2.001350	2.001229	2.820340	2.945543																																																																																																		
8 B	3.159249	1.724131	1.724138	2.712458	1.774063																																																																																																		
9 B	1.604046	3.309780	1.738892	1.753010	1.822171																																																																																																		
10 B	1.604024	1.738902	3.309845	1.753020	2.879880																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Mn	2.945598	0.000000																																																																																																					
8 B	1.774149	2.325893	0.000000																																																																																																				
9 B	2.879904	2.248453	2.771600	0.000000																																																																																																			
10 B	1.822097	2.248600	2.771643	2.755001	0.000000																																																																																																		
 <p>11. -1600.09580738 +28.8</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>2.692181</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.769180</td><td>1.893515</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.917031</td><td>2.968677</td><td>3.277338</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>3.413839</td><td>2.777183</td><td>2.925197</td><td>1.578770</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.394587</td><td>1.793042</td><td>2.958750</td><td>1.807409</td><td>1.596558</td></tr> <tr><td>7 C</td><td>1.536371</td><td>1.561835</td><td>1.697199</td><td>3.208981</td><td>3.535004</td></tr> <tr><td>8 B</td><td>3.023793</td><td>1.831734</td><td>1.787600</td><td>2.655249</td><td>1.580745</td></tr> <tr><td>9 Mn</td><td>2.002522</td><td>3.111435</td><td>2.161887</td><td>2.010705</td><td>1.989198</td></tr> <tr><td>10 B</td><td>1.964857</td><td>1.942127</td><td>2.573794</td><td>1.776886</td><td>2.675207</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 C</td><td>2.869817</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.848692</td><td>2.774179</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Mn</td><td>2.889017</td><td>2.936803</td><td>2.241579</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.949513</td><td>1.676878</td><td>2.739287</td><td>2.500262</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.692181	0.000000				3 B	1.769180	1.893515	0.000000			4 B	2.917031	2.968677	3.277338	0.000000		5 C	3.413839	2.777183	2.925197	1.578770	0.000000	6 B	3.394587	1.793042	2.958750	1.807409	1.596558	7 C	1.536371	1.561835	1.697199	3.208981	3.535004	8 B	3.023793	1.831734	1.787600	2.655249	1.580745	9 Mn	2.002522	3.111435	2.161887	2.010705	1.989198	10 B	1.964857	1.942127	2.573794	1.776886	2.675207		6	7	8	9	10	6 B	0.000000					7 C	2.869817	0.000000				8 B	1.848692	2.774179	0.000000			9 Mn	2.889017	2.936803	2.241579	0.000000		10 B	1.949513	1.676878	2.739287	2.500262	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	2.692181	0.000000																																																																																																					
3 B	1.769180	1.893515	0.000000																																																																																																				
4 B	2.917031	2.968677	3.277338	0.000000																																																																																																			
5 C	3.413839	2.777183	2.925197	1.578770	0.000000																																																																																																		
6 B	3.394587	1.793042	2.958750	1.807409	1.596558																																																																																																		
7 C	1.536371	1.561835	1.697199	3.208981	3.535004																																																																																																		
8 B	3.023793	1.831734	1.787600	2.655249	1.580745																																																																																																		
9 Mn	2.002522	3.111435	2.161887	2.010705	1.989198																																																																																																		
10 B	1.964857	1.942127	2.573794	1.776886	2.675207																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 C	2.869817	0.000000																																																																																																					
8 B	1.848692	2.774179	0.000000																																																																																																				
9 Mn	2.889017	2.936803	2.241579	0.000000																																																																																																			
10 B	1.949513	1.676878	2.739287	2.500262	0.000000																																																																																																		
 <p>12. -1600.09453906 +29.59</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.656444</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.505018</td><td>2.718013</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.615179</td><td>1.778834</td><td>2.969528</td><td>0.000000</td><td></td></tr> <tr><td>5 Mn</td><td>3.145345</td><td>3.149358</td><td>1.972963</td><td>2.503714</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.769374</td><td>1.764811</td><td>2.821282</td><td>1.783842</td><td>2.131766</td></tr> <tr><td>7 B</td><td>2.719981</td><td>1.874343</td><td>1.634603</td><td>2.728629</td><td>2.225700</td></tr> <tr><td>8 B</td><td>1.569663</td><td>2.713536</td><td>1.568872</td><td>2.359383</td><td>2.433709</td></tr> <tr><td>9 B</td><td>1.656854</td><td>1.801044</td><td>1.636335</td><td>2.756656</td><td>3.149477</td></tr> <tr><td>10 B</td><td>3.238351</td><td>3.073339</td><td>3.414722</td><td>1.788698</td><td>1.840188</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>1.742149</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.178523</td><td>2.688844</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.921483</td><td>1.849211</td><td>1.817128</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.782650</td><td>3.103063</td><td>3.280934</td><td>3.938054</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.656444	0.000000				3 C	2.505018	2.718013	0.000000			4 B	1.615179	1.778834	2.969528	0.000000		5 Mn	3.145345	3.149358	1.972963	2.503714	0.000000	6 B	2.769374	1.764811	2.821282	1.783842	2.131766	7 B	2.719981	1.874343	1.634603	2.728629	2.225700	8 B	1.569663	2.713536	1.568872	2.359383	2.433709	9 B	1.656854	1.801044	1.636335	2.756656	3.149477	10 B	3.238351	3.073339	3.414722	1.788698	1.840188		6	7	8	9	10	6 B	0.000000					7 B	1.742149	0.000000				8 B	3.178523	2.688844	0.000000			9 B	2.921483	1.849211	1.817128	0.000000		10 B	1.782650	3.103063	3.280934	3.938054	0.000000
	1	2	3	4	5																																																																																																		
1 C	0.000000																																																																																																						
2 B	1.656444	0.000000																																																																																																					
3 C	2.505018	2.718013	0.000000																																																																																																				
4 B	1.615179	1.778834	2.969528	0.000000																																																																																																			
5 Mn	3.145345	3.149358	1.972963	2.503714	0.000000																																																																																																		
6 B	2.769374	1.764811	2.821282	1.783842	2.131766																																																																																																		
7 B	2.719981	1.874343	1.634603	2.728629	2.225700																																																																																																		
8 B	1.569663	2.713536	1.568872	2.359383	2.433709																																																																																																		
9 B	1.656854	1.801044	1.636335	2.756656	3.149477																																																																																																		
10 B	3.238351	3.073339	3.414722	1.788698	1.840188																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	1.742149	0.000000																																																																																																					
8 B	3.178523	2.688844	0.000000																																																																																																				
9 B	2.921483	1.849211	1.817128	0.000000																																																																																																			
10 B	1.782650	3.103063	3.280934	3.938054	0.000000																																																																																																		

 <p>13. -1600.09280790 +30.7</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>2.885612</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.892137</td><td>1.858186</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.741479</td><td>2.862583</td><td>2.844799</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.973348</td><td>2.628221</td><td>1.849138</td><td>1.848564</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.934485</td><td>1.810208</td><td>2.608589</td><td>1.868338</td><td>1.888469</td></tr> <tr><td>7 C</td><td>1.636855</td><td>1.735710</td><td>1.699627</td><td>2.505844</td><td>2.731530</td></tr> <tr><td>8 C</td><td>3.534302</td><td>1.607503</td><td>1.597854</td><td>2.789687</td><td>1.596539</td></tr> <tr><td>9 Mn</td><td>1.967406</td><td>3.349305</td><td>2.165785</td><td>2.138881</td><td>2.141104</td></tr> <tr><td>10 B</td><td>1.714710</td><td>1.762722</td><td>2.811277</td><td>1.856508</td><td>2.841917</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 C</td><td>2.714695</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>1.605208</td><td>2.636375</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Mn</td><td>3.328532</td><td>2.161029</td><td>3.198513</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.753997</td><td>1.785642</td><td>2.724633</td><td>3.060645</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.885612	0.000000				3 B	2.892137	1.858186	0.000000			4 B	1.741479	2.862583	2.844799	0.000000		5 B	2.973348	2.628221	1.849138	1.848564	0.000000	6 B	2.934485	1.810208	2.608589	1.868338	1.888469	7 C	1.636855	1.735710	1.699627	2.505844	2.731530	8 C	3.534302	1.607503	1.597854	2.789687	1.596539	9 Mn	1.967406	3.349305	2.165785	2.138881	2.141104	10 B	1.714710	1.762722	2.811277	1.856508	2.841917		6	7	8	9	10	6 B	0.000000					7 C	2.714695	0.000000				8 C	1.605208	2.636375	0.000000			9 Mn	3.328532	2.161029	3.198513	0.000000		10 B	1.753997	1.785642	2.724633	3.060645	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	2.885612	0.000000																																																																																																					
3 B	2.892137	1.858186	0.000000																																																																																																				
4 B	1.741479	2.862583	2.844799	0.000000																																																																																																			
5 B	2.973348	2.628221	1.849138	1.848564	0.000000																																																																																																		
6 B	2.934485	1.810208	2.608589	1.868338	1.888469																																																																																																		
7 C	1.636855	1.735710	1.699627	2.505844	2.731530																																																																																																		
8 C	3.534302	1.607503	1.597854	2.789687	1.596539																																																																																																		
9 Mn	1.967406	3.349305	2.165785	2.138881	2.141104																																																																																																		
10 B	1.714710	1.762722	2.811277	1.856508	2.841917																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 C	2.714695	0.000000																																																																																																					
8 C	1.605208	2.636375	0.000000																																																																																																				
9 Mn	3.328532	2.161029	3.198513	0.000000																																																																																																			
10 B	1.753997	1.785642	2.724633	3.060645	0.000000																																																																																																		
 <p>14. -1600.09234750 Cs +31.0</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 C</td><td>1.689214</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.855346</td><td>1.801366</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.602523</td><td>2.610859</td><td>2.761418</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.840000</td><td>1.689040</td><td>1.819396</td><td>1.602492</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.819346</td><td>1.801299</td><td>2.631600</td><td>2.761341</td><td>2.855086</td></tr> <tr><td>7 B</td><td>1.854683</td><td>2.712425</td><td>2.851681</td><td>1.598943</td><td>2.617294</td></tr> <tr><td>8 B</td><td>2.617317</td><td>2.712326</td><td>1.803835</td><td>1.598930</td><td>1.854682</td></tr> <tr><td>9 B</td><td>2.900128</td><td>1.647050</td><td>1.738462</td><td>3.557325</td><td>2.899917</td></tr> <tr><td>10 Mn</td><td>3.313025</td><td>2.910317</td><td>2.137435</td><td>3.228732</td><td>3.313000</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.803863</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.851491</td><td>1.853500</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.738644</td><td>2.985674</td><td>2.985478</td><td>0.000000</td><td></td></tr> <tr><td>10 Mn</td><td>2.137314</td><td>2.195769</td><td>2.195745</td><td>1.958339</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.689214	0.000000				3 B	2.855346	1.801366	0.000000			4 C	1.602523	2.610859	2.761418	0.000000		5 B	1.840000	1.689040	1.819396	1.602492	0.000000	6 B	1.819346	1.801299	2.631600	2.761341	2.855086	7 B	1.854683	2.712425	2.851681	1.598943	2.617294	8 B	2.617317	2.712326	1.803835	1.598930	1.854682	9 B	2.900128	1.647050	1.738462	3.557325	2.899917	10 Mn	3.313025	2.910317	2.137435	3.228732	3.313000		6	7	8	9	10	6 B	0.000000					7 B	1.803863	0.000000				8 B	2.851491	1.853500	0.000000			9 B	1.738644	2.985674	2.985478	0.000000		10 Mn	2.137314	2.195769	2.195745	1.958339	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 C	1.689214	0.000000																																																																																																					
3 B	2.855346	1.801366	0.000000																																																																																																				
4 C	1.602523	2.610859	2.761418	0.000000																																																																																																			
5 B	1.840000	1.689040	1.819396	1.602492	0.000000																																																																																																		
6 B	1.819346	1.801299	2.631600	2.761341	2.855086																																																																																																		
7 B	1.854683	2.712425	2.851681	1.598943	2.617294																																																																																																		
8 B	2.617317	2.712326	1.803835	1.598930	1.854682																																																																																																		
9 B	2.900128	1.647050	1.738462	3.557325	2.899917																																																																																																		
10 Mn	3.313025	2.910317	2.137435	3.228732	3.313000																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	1.803863	0.000000																																																																																																					
8 B	2.851491	1.853500	0.000000																																																																																																				
9 B	1.738644	2.985674	2.985478	0.000000																																																																																																			
10 Mn	2.137314	2.195769	2.195745	1.958339	0.000000																																																																																																		
 <p>15. -1600.09220250 +31.1</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.818638</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.842642</td><td>2.632403</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>2.864651</td><td>2.761827</td><td>2.796380</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.880385</td><td>2.854557</td><td>1.809800</td><td>1.616937</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.854539</td><td>1.774829</td><td>2.851603</td><td>1.605869</td><td>1.872146</td></tr> <tr><td>7 B</td><td>1.685308</td><td>1.724851</td><td>1.717869</td><td>3.553773</td><td>2.892460</td></tr> <tr><td>8 C</td><td>2.482039</td><td>1.744422</td><td>1.831827</td><td>2.660271</td><td>1.770037</td></tr> <tr><td>9 Mn</td><td>2.255999</td><td>3.330047</td><td>2.069176</td><td>1.912856</td><td>2.110398</td></tr> <tr><td>10 B</td><td>1.820881</td><td>1.787018</td><td>2.811674</td><td>1.635182</td><td>2.611931</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.869698</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>1.688443</td><td>1.618795</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Mn</td><td>3.055842</td><td>3.345491</td><td>3.180496</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.870123</td><td>2.905940</td><td>2.698914</td><td>2.213223</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.818638	0.000000				3 B	1.842642	2.632403	0.000000			4 C	2.864651	2.761827	2.796380	0.000000		5 B	2.880385	2.854557	1.809800	1.616937	0.000000	6 B	2.854539	1.774829	2.851603	1.605869	1.872146	7 B	1.685308	1.724851	1.717869	3.553773	2.892460	8 C	2.482039	1.744422	1.831827	2.660271	1.770037	9 Mn	2.255999	3.330047	2.069176	1.912856	2.110398	10 B	1.820881	1.787018	2.811674	1.635182	2.611931		6	7	8	9	10	6 B	0.000000					7 B	2.869698	0.000000				8 C	1.688443	1.618795	0.000000			9 Mn	3.055842	3.345491	3.180496	0.000000		10 B	1.870123	2.905940	2.698914	2.213223	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.818638	0.000000																																																																																																					
3 B	1.842642	2.632403	0.000000																																																																																																				
4 C	2.864651	2.761827	2.796380	0.000000																																																																																																			
5 B	2.880385	2.854557	1.809800	1.616937	0.000000																																																																																																		
6 B	2.854539	1.774829	2.851603	1.605869	1.872146																																																																																																		
7 B	1.685308	1.724851	1.717869	3.553773	2.892460																																																																																																		
8 C	2.482039	1.744422	1.831827	2.660271	1.770037																																																																																																		
9 Mn	2.255999	3.330047	2.069176	1.912856	2.110398																																																																																																		
10 B	1.820881	1.787018	2.811674	1.635182	2.611931																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	2.869698	0.000000																																																																																																					
8 C	1.688443	1.618795	0.000000																																																																																																				
9 Mn	3.055842	3.345491	3.180496	0.000000																																																																																																			
10 B	1.870123	2.905940	2.698914	2.213223	0.000000																																																																																																		



16. -1600.08705638 +34.3

	1	2	3	4	5
1 B	0.000000				
2 B	2.875389	0.000000			
3 B	2.853408	2.883120	0.000000		
4 B	1.778236	2.872836	2.906887	0.000000	
5 C	2.740921	2.742304	1.735996	1.718668	0.000000
6 B	2.889719	1.769252	2.903779	1.793319	1.704482
7 Mn	1.991936	1.999669	1.963638	2.958209	2.800149
8 B	3.288745	1.727466	1.721721	2.858955	1.699077
9 C	1.633863	3.146883	1.642706	1.742516	1.635612
10 B	1.718161	1.737756	3.313891	1.766285	2.715935
	6	7	8	9	10
6 B	0.000000				
7 Mn	2.955111	0.000000			
8 B	1.796569	2.280379	0.000000		
9 C	2.736924	2.165689	2.621684	0.000000	
10 B	1.803532	2.317293	2.782880	2.632438	0.000000

Table 3. Energy ranking

	Initial structure	Final energy (a.u.)	D kcal/mole	Remarks
1	1-TetrTriPri1_Mn_v6_C2_v36b	-1600.14169157	0.00	
2	2-TetrTriPri2_Mn_v3_C2_v66a	-1600.14168889	0.00	
3	2-TetrTriPri2_Mn_v3_C2_v66b	-1600.14168881	0.00	
4	2-TetrTriPri2_Mn_v4_C2_v65c	-1600.14168881	0.00	
5	1-TetrTriPri1_Mn_v6_C2_v65a	-1600.14168878	0.00	
6	2-TetrTriPri2_Mn_v6_C2_v44b_r-36	-1600.14168878	0.00	
7	7-Isocloso_Mn_v6_C2_v2_c	-1600.14168878	0.00	
8	7-Isocloso_Mn_v6_C2_v2_r_r-36	-1600.14168878	0.00	
9	2-TetrTriPri2_Mn_v6_C2_v34a	-1600.14168874	0.00	
10	6-AntiPr-Mn_v4_C2_v2_j	-1600.14168850	0.00	
11	2-TetrTriPri2_Mn_v5_C2_v55	-1600.14168837	0.00	
12	7-Isocloso_Mn_v5b_C2_t	-1600.14168837	0.00	
13	7-Isocloso_Mn_v4_C2_m	-1600.14168799	0.00	
14	1-TetrTriPri1_Mn_v6_C2_v35d	-1600.14108114	0.38	
15	2-TetrTriPri2_Mn_v6_C2_v44b_i-36	-1600.14089842	0.50	
16	7-Isocloso_Mn_v6_C2_v2_r	-1600.14089839	0.50	
17	2-TetrTriPri2_Mn_v6_C2_v46	-1600.13831317	2.12	
18	2-TetrTriPri2_Mn_v3_C2_v64b	-1600.13831304	2.12	
19	7-Isocloso_Mn_v6_C2_v2_s	-1600.13831296	2.12	
20	1-TetrTriPri1_Mn_v6_C2_v33	-1600.13831105	2.12	
21	7-Isocloso_Mn_v4_C2_a_r-18	-1600.13830915	2.12	
22	7-Isocloso_Mn_v4_C2_a_i-18	-1600.13828743	2.13	
23	2-TetrTriPri2_Mn_v3_C2_v46c_r-19	-1600.13826752	2.15	
24	1-TetrTriPri1_Mn_v6_C2_v65c_r-19	-1600.13826679	2.15	
25	2-TetrTriPri2_Mn_v6_C2_v35a_r-18	-1600.13824996	2.16	
26	7-Isocloso_Mn_v6_C2_v2_b_r-17	-1600.13824990	2.16	
27	1-TetrTriPri1_Mn_v6_C2_v65c_i-19	-1600.13820982	2.18	
28	2-TetrTriPri2_Mn_v3_C2_v46c_i-19	-1600.13820657	2.19	
29	2-TetrTriPri2_Mn_v6_C2_v35a_i-18	-1600.13820059	2.19	
30	7-Isocloso_Mn_v6_C2_v2_b_i-17	-1600.13820025	2.19	
31	2-TetrTriPri2_Mn_v3_C2_v44b	-1600.12510354	10.41	
32	4-BicapSqAntipr_Mn_v5_C2_r_r-30	-1600.12510350	10.41	
33	7-Isocloso_Mn_v5b_C2_q_r-31	-1600.12510328	10.41	
34	2-TetrTriPri2_Mn_v5_C2_v65a	-1600.12510312	10.41	
35	7-Isocloso_Mn_v6_C2_v2_u	-1600.12510290	10.41	
36	2-TetrTriPri2_Mn_v6_C2_v66	-1600.12510280	10.41	
37	2-TetrTriPri2_Mn_v6_C2_v55a	-1600.12510174	10.41	
38	2-TetrTriPri2_Mn_v3_C2_v44a	-1600.12510002	10.41	

39	7-Isocloso_Mn_v6_C2_v2_k	-1600.12505770	10.44	
40	4-BicapSqAntipr_Mn_v5_C2_r i-30	-1600.12435979	10.87	
41	7-Isocloso_Mn_v5b_C2_q i-31	-1600.12435592	10.88	
42	7-Isocloso_Mn_v4_C2_n	-1600.12070015	13.17	
43	7-Isocloso_Mn_v5b_C2_b_r-1523	-1600.12070015	13.17	
44	7-Isocloso_Mn_v5b_C2_b_r-30	-1600.12070013	13.17	
45	7-Isocloso_Mn_v5a_C2_n	-1600.12070009	13.17	
46	2-TetrTriPri2_Mn_v5_C2_v64c	-1600.12069895	13.17	
47	2-TetrTriPri2_Mn_v4_C2_v46b	-1600.12067724	13.18	
48	4-BicapSqAntipr_Mn_v5_C2_a	-1600.12067423	13.19	
49	1-TetrTriPri1_Mn_v6_C2_v65b	-1600.11976890	13.75	
50	1-TetrTriPri1_Mn_v6_C2_v35c	-1600.11976384	13.76	
51	1-TetrTriPri1_Mn_v6_C2_v45a	-1600.11976361	13.76	
52	2-TetrTriPri2_Mn_v6_C2_v45e	-1600.11976316	13.76	
53	7-Isocloso_Mn_v6_C2_v2_q	-1600.11976285	13.76	
54	2-TetrTriPri2_Mn_v6_C2_v44a	-1600.11976250	13.76	
55	1-TetrTriPri1_Mn_v6_C2_v65d	-1600.11976221	13.76	
56	3-BicapCub_Mn_v4b_C2_o	-1600.11976218	13.76	
57	2-TetrTriPri2_Mn_v3_C2_v55a	-1600.11976210	13.76	
58	6-AntiPr-Mn_v4_C2_v2_d	-1600.11976203	13.76	
59	3-BicapCub_Mn_v4b_C2_n	-1600.11976182	13.76	
60	2-TetrTriPri2_Mn_v3_C2_v56b	-1600.11976105	13.76	
61	1-TetrTriPri1_Mn_v4_C2_v55c	-1600.11976055	13.76	
62	1-TetrTriPri1_Mn_v4_C2_v45b	-1600.11975990	13.76	
63	7-Isocloso_Mn_v6_C2_v2_e	-1600.11975886	13.76	
64	7-Isocloso_Mn_v6_C2_v2_i	-1600.11975882	13.76	
65	2-TetrTriPri2_Mn_v3_C2_v65a	-1600.11975695	13.76	
66	7-Isocloso_Mn_v4_C2_e_r-25	-1600.11975573	13.76	
67	7-Isocloso_Mn_v4_C2_e	-1600.11905784	14.20	
68	7-Isocloso_Mn_v6_C2_v2_p	-1600.11030842	19.69	
69	2-TetrTriPri2_Mn_v6_C2_v56a	-1600.11030817	19.69	
70	7-Isocloso_Mn_v6_C2_v2_f_r-26	-1600.11030807	19.69	
71	2-TetrTriPri2_Mn_v6_C2_v54a_r-25	-1600.11030794	19.69	
72	2-TetrTriPri2_Mn_v3_C2_v54a	-1600.11030793	19.69	
73	2-TetrTriPri2_Mn_v3_C2_v54d	-1600.11030788	19.69	
74	7-Isocloso_Mn_v5b_C2_f	-1600.11030678	19.69	
75	7-Isocloso_Mn_v4_C2_f	-1600.11030626	19.69	
76	7-Isocloso_Mn_v6_C2_v2_f i-26	-1600.10982226	20.00	
77	2-TetrTriPri2_Mn_v6_C2_v54a i-25	-1600.10982214	20.00	
78	2-TetrTriPri2_Mn_v3_C2_v64a	-1600.10947096	20.22	C-C
79	2-TetrTriPri2_Mn_v6_C2_v45d	-1600.10946617	20.22	C-C

80	2-TetrTriPri2_Mn_v3_C2_v46b	-1600.10946568	20.22	C-C
81	7-Isocloso_Mn_v6_C2_v2_t	-1600.10946424	20.22	C-C
82	1-TetrTriPri1_Mn_v6_C2_v36a	-1600.10946389	20.22	C-C
83	2-TetrTriPri2_Mn_v3_C2_v46a	-1600.10946369	20.22	C-C
84	2-TetrTriPri2_Mn_v6_C2_v54b	-1600.10946316	20.22	C-C
85	2-TetrTriPri2_Mn_v6_C2_v36	-1600.10946283	20.22	C-C
86	7-Isocloso_Mn_v4_C2_g	-1600.10946248	20.22	C-C
87	1-TetrTriPri1_Mn_v6_C2_v35a	-1600.10946159	20.22	C-C
88	7-Isocloso_Mn_v4_C2_d	-1600.10946153	20.22	C-C
89	7-Isocloso_Mn_v6_C2_v2_j	-1600.10946131	20.22	C-C
90	4-BicapSqAntipr_Mn_v5_C2_d	-1600.10946052	20.22	C-C
91	7-Isocloso_Mn_v6_C2_v2_d	-1600.10945969	20.22	C-C
92	2-TetrTriPri2_Mn_v4_C2_v45a	-1600.10945580	20.23	C-C
93	7-Isocloso_Mn_v5b_C2_b -1523 -30	-1600.10727978	21.59	
94	1-TetrTriPri1_Mn_v4_C2_v34b	-1600.10092144	25.58	
95	7-Isocloso_Mn_v5b_C2_d	-1600.09809624	27.35	
96	2-TetrTriPri2_Mn_v5_C2_v45b	-1600.09809167	27.36	
97	4-BicapSqAntipr_Mn_v5_C2_c	-1600.09809164	27.36	
98	7-Isocloso_Mn_v5a_C2_o	-1600.09809162	27.36	
99	2-TetrTriPri2_Mn_v4_C2_v65d_r-16	-1600.09809161	27.36	
100	7-Isocloso_Mn_v4_C2_c_r-15	-1600.09809158	27.36	
101	2-TetrTriPri2_Mn_v4_C2_v66b	-1600.09808798	27.36	
102	7-Isocloso_Mn_v4_C2_c_i-15	-1600.09805990	27.38	
103	2-TetrTriPri2_Mn_v4_C2_v65d_i-16	-1600.09792824	27.46	
104	7-Isocloso_Mn_v5b_C2_a_r-35	-1600.09771771	27.59	C-C
105	4-BicapSqAntipr_Mn_v5_C2_b_r-35	-1600.09771724	27.59	C-C
106	2-TetrTriPri2_Mn_v3_C2_v56c	-1600.09771710	27.59	C-C
107	2-TetrTriPri2_Mn_v3_C2_v65b	-1600.09771709	27.59	C-C
108	7-Isocloso_Mn_v4_C2_b_r-35	-1600.09771708	27.59	C-C
109	7-Isocloso_Mn_v6_C2_v2_n	-1600.09771706	27.59	C-C
110	7-Isocloso_Mn_v6_C2_v2_a	-1600.09771677	27.59	C-C
111	2-TetrTriPri2_Mn_v6_C2_v34b	-1600.09771657	27.59	C-C
112	2-TetrTriPri2_Mn_v6_C2_v45c	-1600.09771608	27.59	C-C
113	7-Isocloso_Mn_v4_C2_b_i-35	-1600.09688919	28.11	C-C
114	4-BicapSqAntipr_Mn_v5_C2_b_i-35	-1600.09688906	28.11	C-C
115	7-Isocloso_Mn_v5b_C2_a_i-35	-1600.09688899	28.11	C-C
116	2-TetrTriPri2_Mn_v4_C2_v35b	-1600.09580738	28.79	
117	3-BicapCub_Mn_v4b_C2_v	-1600.09580737	28.79	
118	3-BicapCub_Mn_v4b_C2_i	-1600.09580723	28.79	
119	3-BicapCub_Mn_v4b_C2_c	-1600.09580716	28.79	
120	6-AntiPr-Mn_v4_C2_v2_h	-1600.09580691	28.79	

121	6-AntiPr-Mn_v4_C2_v2_o	-1600.09580649	28.79	
122	1-TetrTriPri1_Mn_v4_C2_v65b	-1600.09453906	29.59	
123	4-BicapSqAntipr_Mn_v5_C2_p	-1600.09453897	29.59	
124	3-BicapCub_Mn_v4b_C2_t	-1600.09453895	29.59	
125	5-PentagPrism_Mn_v3_m	-1600.09453890	29.59	
126	7-Isocloso_Mn_v5a_C2_j	-1600.09453890	29.59	
127	7-Isocloso_Mn_v5b_C2_k	-1600.09453884	29.59	
128	3-BicapCub_Mn_v4b_C2_x	-1600.09453879	29.59	
129	7-Isocloso_Mn_v5a_C2_g	-1600.09453851	29.59	
130	2-TetrTriPri2_Mn_v5_C2_v45a	-1600.09453833	29.59	
131	2-TetrTriPri2_Mn_v5_C2_v34b	-1600.09453831	29.59	
132	2-TetrTriPri2_Mn_v4_C2_v34	-1600.09280790	30.67	
133	7-Isocloso_Mn_v4_C2_h	-1600.09280608	30.67	
134	7-Isocloso_Mn_v5a_C2_d	-1600.09280519	30.67	
135	2-TetrTriPri2_Mn_v5_C2_v65b	-1600.09280518	30.67	
136	2-TetrTriPri2_Mn_v5_C2_v66a	-1600.09280489	30.67	
137	4-BicapSqAntipr_Mn_v5_C2_h	-1600.09280473	30.67	
138	7-Isocloso_Mn_v5a_C2_s	-1600.09279099	30.68	
139	7-Isocloso_Mn_v4_C2_s	-1600.09234750	30.96	
140	4-BicapSqAntipr_Mn_v5_C2_f	-1600.09234636	30.96	
141	2-TetrTriPri2_Mn_v4_C2_v44	-1600.09229080	31.00	
142	2-TetrTriPri2_Mn_v4_C2_v65a	-1600.09227654	31.01	
143	2-TetrTriPri2_Mn_v4_C2_v45b	-1600.09220250	31.05	
144	7-Isocloso_Mn_v4_C2_l	-1600.09220245	31.05	
145	2-TetrTriPri2_Mn_v5_C2_v65c	-1600.09220242	31.05	
146	7-Isocloso_Mn_v4_C2_o	-1600.09220241	31.05	
147	7-Isocloso_Mn_v5b_C2_l	-1600.09220172	31.05	
148	7-Isocloso_Mn_v5b_C2_g	-1600.09220076	31.05	
149	2-TetrTriPri2_Mn_v5_C2_v44a	-1600.09219850	31.06	
150	4-BicapSqAntipr_Mn_v5_C2_e	-1600.09219470	31.06	
151	2-TetrTriPri2_Mn_v4_C2_v66a	-1600.09219160	31.06	
152	2-TetrTriPri2_Mn_v4_C2_v56a	-1600.09217458	31.07	
153	2-TetrTriPri2_Mn_v3_C2_v54b	-1600.08705638	34.28	C-C
154	2-TetrTriPri2_Mn_v6_C2_v45b	-1600.08705637	34.28	C-C
155	7-Isocloso_Mn_v6_C2_v2_m	-1600.08705048	34.29	C-C
156	2-TetrTriPri2_Mn_v3_C2_v45a	-1600.08704847	34.29	C-C
157	7-Isocloso_Mn_v6_C2_v2_l	-1600.08704807	34.29	C-C
158	2-TetrTriPri2_Mn_v3_C2_v54c	-1600.08704594	34.29	C-C
159	2-TetrTriPri2_Mn_v6_C2_v55b	-1600.08704518	34.29	C-C
160	7-Isocloso_Mn_v6_C2_v2_h	-1600.08703878	34.29	C-C
161	1-TetrTriPri1_Mn_v6_C2_v46	-1600.08703855	34.29	C-C

162	1-TetrTriPri1_Mn_v6_C2_v35b	-1600.08702390	34.30	C-C
163	6-AntiPr-Mn_v4_C2_v2_p	-1600.08393274	36.24	
164	3-BicapCub_Mn_v4b_C2_d	-1600.08393225	36.24	
165	5-PentagPrism_Mn_v3_r	-1600.08393213	36.24	
166	2-TetrTriPri2_Mn_v3_C2_v55c	-1600.08308417	36.77	
167	2-TetrTriPri2_Mn_v5_C2_v66b	-1600.08308414	36.77	
168	4-BicapSqAntipr_Mn_v5_C2_m	-1600.08308405	36.77	
169	7-Isocloso_Mn_v5b_C2_u	-1600.08308399	36.77	
170	7-Isocloso_Mn_v5a_C2_r	-1600.08308395	36.77	
171	3-BicapCub_Mn_v4b_C2_k	-1600.08298192	36.84	
172	3-BicapCub_Mn_v4b_C2_r	-1600.08298189	36.84	
173	6-AntiPr-Mn_v4_C2_v2_i	-1600.08298189	36.84	
174	3-BicapCub_Mn_v4b_C2_e	-1600.08265015	37.05	C-C
175	6-AntiPr-Mn_v4_C2_v2_e	-1600.08265013	37.05	C-C
176	5-PentagPrism_Mn_v3_q	-1600.08264947	37.05	C-C
177	7-Isocloso_Mn_v4_C2_r	-1600.08187779	37.53	
178	6-AntiPr-Mn_v4_C2_v2_r	-1600.07837672	39.73	
179	3-BicapCub_Mn_v4b_C2_l	-1600.07790892	40.02	
180	6-AntiPr-Mn_v4_C2_v2_c	-1600.07790888	40.02	
181	2-TetrTriPri2_Mn_v6_C2_v56b	-1600.07695375	40.62	
182	3-BicapCub_Mn_v4a_C2_f	-1600.07641100	40.96	
183	4-BicapSqAntipr_Mn_v4_C2_h_r-25	-1600.07635852	40.99	
184	2-TetrTriPri2_Mn_v4_C2_v65b	-1600.07630256	41.03	
185	4-BicapSqAntipr_Mn_v4_C2_h	-1600.07580362	41.34	
186	7-Isocloso_Mn_v5b_C2_o	-1600.07376997	42.62	
187	4-BicapSqAntipr_Mn_v5_C2_j	-1600.07376275	42.62	
188	7-Isocloso_Mn_v5b_C2_s	-1600.07376260	42.62	
189	3-BicapCub_Mn_v4b_C2_h	-1600.07357156	42.74	
190	6-AntiPr-Mn_v4_C2_v2_s_r-26	-1600.07357121	42.74	
191	6-AntiPr-Mn_v4_C2_v2_s_i-26	-1600.07348628	42.80	
192	7-Isocloso_Mn_v5a_C2_c_r-54	-1600.07285950	43.19	
193	1-TetrTriPri1_Mn_v6_C2_v55b	-1600.07275609	43.26	
194	7-Isocloso_Mn_v5a_C2_e	-1600.07264808	43.32	
195	7-Isocloso_Mn_v5b_C2_p_r-24	-1600.07264805	43.32	
196	4-BicapSqAntipr_Mn_v5_C2_s	-1600.07264804	43.32	
197	7-Isocloso_Mn_v5b_C2_p_i-24	-1600.07198970	43.74	
198	3-BicapCub_Mn_v4b_C2_s	-1600.07120235	44.23	
199	5-PentagPrism_Mn_v3_a	-1600.07118374	44.24	
200	6-AntiPr-Mn_v4_C2_v2_n	-1600.07118349	44.24	
201	1-TetrTriPri1_Mn_v6_C2_v55a	-1600.07110884	44.29	
202	1-TetrTriPri1_Mn_v4_C2_v33	-1600.07104015	44.33	

203	5-PentagPrism_Mn_v3_k	-1600.07103981	44.33	
204	2-TetrTriPri2_Mn_v6_C2_v35b	-1600.07103943	44.33	
205	7-Isocloso_Mn_v4_C2_q	-1600.07096753	44.38	
206	2-TetrTriPri2_Mn_v5_C2_v64b	-1600.07095879	44.38	C-C
207	7-Isocloso_Mn_v5b_C2_m	-1600.07094707	44.39	C-C
208	7-Isocloso_Mn_v5b_C2_c	-1600.07091632	44.41	C-C
209	7-Isocloso_Mn_v5a_C2_c i-54	-1600.07058631	44.62	
210	2-TetrTriPri2_Mn_v3_C2_v55b	-1600.07025051	44.83	C-C
211	7-Isocloso_Mn_v4_C2_u	-1600.07025010	44.83	C-C
212	2-TetrTriPri2_Mn_v6_C2_v45a	-1600.07024914	44.83	C-C
213	7-Isocloso_Mn_v6_C2_v2_g	-1600.07013564	44.90	C-C
214	7-Isocloso_Mn_v6_C2_v2_o r-20-13	-1600.07005063	44.95	C-C
215	1-TetrTriPri1_Mn_v4_C2_v65a	-1600.06998551	44.99	
216	7-Isocloso_Mn_v6_C2_v2_o r-20	-1600.06997911	45.00	C-C
217	7-Isocloso_Mn_v6_C2_v2_o i-20	-1600.06993514	45.03	C-C
218	3-BicapCub_Mn_v4b_C2_b	-1600.06935942	45.39	
219	7-Isocloso_Mn_v4_C2_p	-1600.06784015	46.34	C-C
220	7-Isocloso_Mn_v5b_C2_n	-1600.06783985	46.34	C-C
221	2-TetrTriPri2_Mn_v4_C2_v46a	-1600.06783287	46.34	C-C
222	1-TetrTriPri1_Mn_v4_C2_v45c	-1600.06718179	46.75	
223	7-Isocloso_Mn_v5a_C2_q	-1600.06631552	47.30	C-C
224	2-TetrTriPri2_Mn_v5_C2_v64d	-1600.06631345	47.30	C-C
225	4-BicapSqAntipr_Mn_v5_C2_i	-1600.06631216	47.30	C-C
226	7-Isocloso_Mn_v5a_C2_t	-1600.06631113	47.30	C-C
227	1-TetrTriPri1_Mn_v4_C2_v44	-1600.06624083	47.34	
228	4-BicapSqAntipr_Mn_v5_C2_n	-1600.06587699	47.57	
229	5-PentagPrism_Mn_v3_j	-1600.06568016	47.70	
230	7-Isocloso_Mn_v5b_C2_h	-1600.06561351	47.74	
231	7-Isocloso_Mn_v5a_C2_l	-1600.06555412	47.77	
232	5-PentagPrism_Mn_v3_i	-1600.06543894	47.85	
233	3-BicapCub_Mn_v4b_C2_w	-1600.06488656	48.19	
234	6-AntiPr-Mn_v4_C2_v2_g	-1600.06488616	48.19	
235	2-TetrTriPri2_Mn_v5_C2_v35	-1600.06373007	48.92	
236	7-Isocloso_Mn_v5a_C2_i	-1600.06372974	48.92	
237	5-PentagPrism_Mn_v3_o	-1600.06368083	48.95	
238	4-BicapSqAntipr_Mn_v5_C2_o	-1600.06367212	48.96	
239	7-Isocloso_Mn_v5a_C2_m	-1600.06366865	48.96	
240	2-TetrTriPri2_Mn_v5_C2_v44b	-1600.06366796	48.96	
241	1-TetrTriPri1_Mn_v4_C2_v45d	-1600.06135863	50.41	
242	1-TetrTriPri1_Mn_v6_C2_v43	-1600.06081552	50.75	
243	2-TetrTriPri2_Mn_v5_C2_v36	-1600.06053507	50.92	C-C

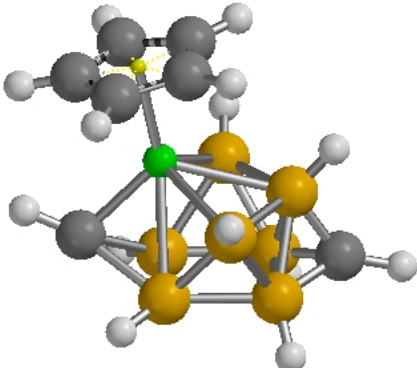
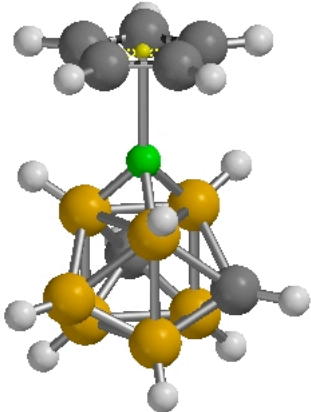
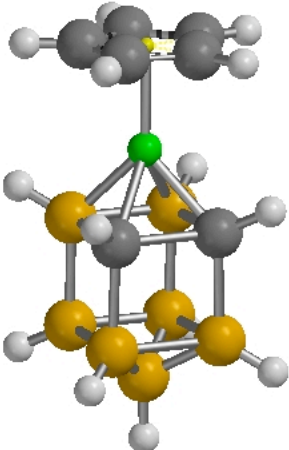
244	2-TetrTriPri2_Mn_v5_C2_v46a	-1600.06053470	50.92	C-C
245	7-Isocloso_Mn_v4_C2_k	-1600.06053464	50.92	C-C
246	7-Isocloso_Mn_v4_C2_t	-1600.06053457	50.92	C-C
247	2-TetrTriPri2_Mn_v4_C2_v64a	-1600.06053455	50.92	C-C
248	7-Isocloso_Mn_v5a_C2_k	-1600.06053418	50.92	C-C
249	2-TetrTriPri2_Mn_v4_C2_v54a	-1600.06053415	50.92	C-C
250	4-BicapSqAntipr_Mn_v5_C2_g	-1600.06053405	50.92	C-C
251	7-Isocloso_Mn_v5a_C2_h	-1600.06053092	50.93	C-C
252	3-BicapCub_Mn_v4b_C2_f	-1600.05980833	51.38	
253	1-TetrTriPri1_Mn_v6_C2_v55c	-1600.05911333	51.82	C-C
254	5-PentagPrism_Mn_v3_t	-1600.05773497	52.68	
255	1-TetrTriPri1_Mn_v6_C2_v66	-1600.05773477	52.68	
256	5-PentagPrism_Mn_v3_p	-1600.05773475	52.68	
257	3-BicapCub_Mn_v4b_C2_p	-1600.05716114	53.04	C-C
258	5-PentagPrism_Mn_v3_l	-1600.05716092	53.04	C-C
259	7-Isocloso_Mn_v5a_C2_p	-1600.05401998	55.01	C-C
260	2-TetrTriPri2_Mn_v5_C2_v45c	-1600.05401992	55.01	C-C
261	5-PentagPrism_Mn_v3_g	-1600.05121346	56.77	C-C
262	1-TetrTriPri1_Mn_v4_C2_v36b	-1600.05109234	56.85	
263	5-PentagPrism_Mn_v3_n	-1600.05096386	56.93	C-C
264	4-BicapSqAntipr_Mn_v5_C2_t_r-19	-1600.05021289	57.40	C-C
265	4-BicapSqAntipr_Mn_v5_C2_t_i-19	-1600.04994529	57.57	C-C
266	5-PentagPrism_Mn_v3_s	-1600.04839925	58.54	
267	2-TetrTriPri2_Mn_v4_C2_v55b	-1600.04839018	58.54	
268	5-PentagPrism_Mn_v3_d	-1600.04822533	58.65	
269	6-AntiPr-Mn_v4_C2_v2_m	-1600.04787333	58.87	C-C
270	7-Isocloso_Mn_v5b_C2_e	-1600.04760240	59.04	
271	2-TetrTriPri2_Mn_v4_C2_v55a	-1600.04759985	59.04	
272	7-Isocloso_Mn_v5b_C2_r	-1600.04742121	59.15	C-C
273	4-BicapSqAntipr_Mn_v5_C2_k	-1600.04742087	59.15	C-C
274	7-Isocloso_Mn_v5a_C2_b	-1600.04717343	59.31	
275	2-TetrTriPri2_Mn_v5_C2_v64a	-1600.04717302	59.31	
276	4-BicapSqAntipr_Mn_v4_C2_f_r-29	-1600.04712712	59.34	
277	3-BicapCub_Mn_v4a_C2_e	-1600.04712700	59.34	
278	3-BicapCub_Mn_v4a_C2_d	-1600.04712290	59.34	
279	4-BicapSqAntipr_Mn_v4_C2_g_r-28	-1600.04712281	59.34	
280	1-TetrTriPri1_Mn_v4_C2_v64	-1600.04708284	59.37	
281	4-BicapSqAntipr_Mn_v4_C2_g_i-28	-1600.04664136	59.64	
282	4-BicapSqAntipr_Mn_v4_C2_f_i-29	-1600.04663871	59.64	
283	1-TetrTriPri1_Mn_v4_C2_v35d_r-107	-1600.04621185	59.91	
284	6-AntiPr-Mn_v4_C2_v2_l	-1600.04617264	59.94	C-C

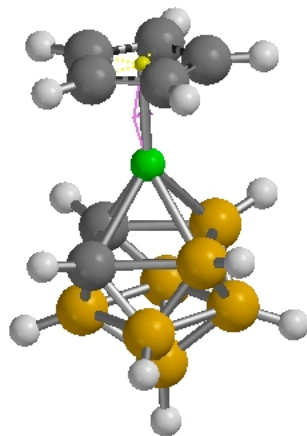
285	3-BicapCub_Mn_v4b_C2_a	-1600.04617229	59.94	
286	1-TetrTriPri1_Mn_v4_C2_v35d i-107	-1600.04603797	60.02	
287	3-BicapCub_Mn_v4a_C2_g	-1600.04463289	60.90	C-C
288	4-BicapSqAntipr_Mn_v4_C2_l r-17	-1600.04460691	60.92	C-C
289	4-BicapSqAntipr_Mn_v4_C2_k r-17	-1600.04458478	60.93	C-C
290	4-BicapSqAntipr_Mn_v4_C2_k i-17	-1600.04455412	60.95	C-C
291	4-BicapSqAntipr_Mn_v4_C2_l i-17	-1600.04455412	60.95	C-C
292	3-BicapCub_Mn_v4a_C2_b	-1600.04445107	61.02	
293	4-BicapSqAntipr_Mn_v4_C2_c	-1600.04439014	61.05	
294	1-TetrTriPri1_Mn_v4_C2_v35c	-1600.04330876	61.73	C-C
295	4-BicapSqAntipr_Mn_v5_C2_q	-1600.04322377	61.79	
296	7-Isocloso_Mn_v5a_C2_a r-357	-1600.04322292	61.79	C-C
297	2-TetrTriPri2_Mn_v5_C2_v63_r-357	-1600.04322287	61.79	C-C
298	2-TetrTriPri2_Mn_v4_C2_v36a	-1600.04322225	61.79	C-C
299	7-Isocloso_Mn_v4_C2_i	-1600.04322205	61.79	C-C
300	1-TetrTriPri1_Mn_v4_C2_v36a	-1600.04263182	62.16	
301	4-BicapSqAntipr_Mn_v5_C2_l	-1600.04173208	62.72	C-C
302	6-AntiPr-Mn_v4_C2_v2_a	-1600.04173129	62.72	C-C
303	7-Isocloso_Mn_v4_C2_j	-1600.04173112	62.72	C-C
304	7-Isocloso_Mn_v5b_C2_i	-1600.04173078	62.72	C-C
305	1-TetrTriPri1_Mn_v4_C2_v55d	-1600.04109109	63.13	
306	2-TetrTriPri2_Mn_v6_C2_v55c	-1600.04109011	63.13	
307	5-PentagPrism_Mn_v3_c	-1600.04094806	63.21	
308	5-PentagPrism_Mn_v3_h	-1600.03932583	64.23	C-C
309	3-BicapCub_Mn_v4b_C2_q	-1600.03863209	64.67	C-C
310	5-PentagPrism_Mn_v3_e	-1600.03835951	64.84	C-C
311	1-TetrTriPri1_Mn_v4_C2_v35b	-1600.03784789	65.16	
312	5-PentagPrism_Mn_v3_f	-1600.03784715	65.16	
313	3-BicapCub_Mn_v4b_C2_m	-1600.03782652	65.17	C-C
314	6-AntiPr-Mn_v4_C2_v2_q	-1600.03685483	65.78	C-C
315	6-AntiPr-Mn_v4_C2_v2_f	-1600.03685466	65.78	C-C
316	3-BicapCub_Mn_v4b_C2_j	-1600.03685377	65.78	C-C
317	4-BicapSqAntipr_Mn_v4_C2_j	-1600.03600502	66.32	
318	4-BicapSqAntipr_Mn_v4_C2_m	-1600.03600502	66.32	
319	3-BicapCub_Mn_v4a_C2_i	-1600.03598936	66.33	
320	2-TetrTriPri2_Mn_v4_C2_v35a	-1600.03598639	66.33	
321	7-Isocloso_Mn_v5a_C2_f r-86	-1600.03508880	66.89	C-C
322	2-TetrTriPri2_Mn_v5_C2_v34a_r-90	-1600.03507529	66.90	C-C
323	1-TetrTriPri1_Mn_v4_C2_v45a	-1600.03359207	67.83	C-C
324	2-TetrTriPri2_Mn_v5_C2_v34a i-90	-1600.03037572	69.85	C-C
325	7-Isocloso_Mn_v5a_C2_f i-86	-1600.03037555	69.85	C-C

326	3-BicapCub_Mn_v4a_C2_a	-1600.02697131	71.99	C-C
327	4-BicapSqAntipr_Mn_v4_C2_b	-1600.02697129	71.99	C-C
328	4-BicapSqAntipr_Mn_v4_C2_a	-1600.02697114	71.99	C-C
329	1-TetrTriPri1_Mn_v6_C2_v45b_r-16	-1600.02556589	72.87	C-C
330	1-TetrTriPri1_Mn_v6_C2_v45b_i-16	-1600.02506058	73.18	C-C
331	4-BicapSqAntipr_Mn_v4_C2_d_r-31	-1600.02471715	73.40	C-C
332	3-BicapCub_Mn_v4a_C2_c	-1600.02471675	73.40	C-C
333	4-BicapSqAntipr_Mn_v4_C2_e_r-31	-1600.02470633	73.41	C-C
334	4-BicapSqAntipr_Mn_v4_C2_d_i-31	-1600.02410458	73.78	C-C
335	4-BicapSqAntipr_Mn_v4_C2_e_i-31	-1600.02410458	73.78	C-C
336	7-Isocloso_Mn_v5b_C2_j	-1600.02313918	74.39	C-C
337	1-TetrTriPri1_Mn_v6_C2_v55d	-1600.02305532	74.44	C-C
338	7-Isocloso_Mn_v5a_C2_u	-1600.02195711	75.13	C-C
339	3-BicapCub_Mn_v4b_C2_g-cont	-1600.02163090	75.34	C-C
340	6-AntiPr-Mn_v4_C2_v2_b	-1600.02163048	75.34	C-C
341	4-BicapSqAntipr_Mn_v4_C2_i_r-10	-1600.02074762	75.89	
342	4-BicapSqAntipr_Mn_v4_C2_i_i-10	-1600.02073923	75.90	
343	2-TetrTriPri2_Mn_v4_C2_v36b	-1600.01928181	76.81	C-C
344	5-PentagPrism_Mn_v3_b	-1600.01636556	78.64	C-C
345	7-Isocloso_Mn_v5a_C2_a_i-357	-1600.01596316	78.89	C-C
346	2-TetrTriPri2_Mn_v5_C2_v63_i-357	-1600.01596294	78.89	C-C
347	6-AntiPr-Mn_v4_C2_v2_k	-1600.01317798	80.64	C-C
348	3-BicapCub_Mn_v4b_C2_u	-1600.01317309	80.64	C-C
349	1-TetrTriPri1_Mn_v4_C2_v34a	-1600.00294271	87.06	
350	1-TetrTriPri1_Mn_v4_C2_v55b	-1599.99693565	90.83	C-C
351	6-AntiPr-Mn_v4_C2_v2_t	-1599.99284281	93.40	C-C
352	3-BicapCub_Mn_v4a_C2_h	-1599.99274657	93.46	C-C
353	1-TetrTriPri1_Mn_v4_C2_v35a	-1599.99153416	94.22	C-C
354	1-TetrTriPri1_Mn_v4_C2_v55a	-1599.97263987	106.08	

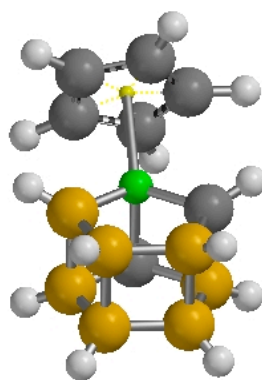
10-vertex $\text{CpReC}_2\text{B}_7\text{H}_9$

Table 1. Initial structures (one example from each family) 316 structures in total

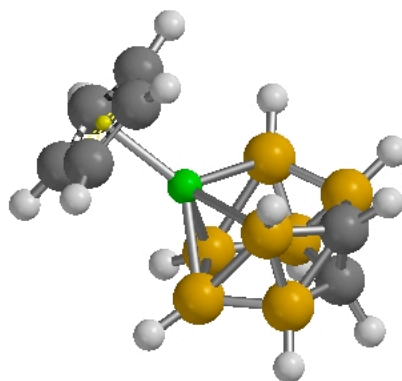
Initial structures
 <p>1. Tetracapped trigonal prism 41 structures</p>
 <p>2. Tetracapped trigonal prism 84 structures</p>
 <p>3. Bicapped cube 33 structures</p>



4. Bicapped square antiprism 34 structures



5. Pentacapped prism 20 structures



6. Antiprism 20 structures

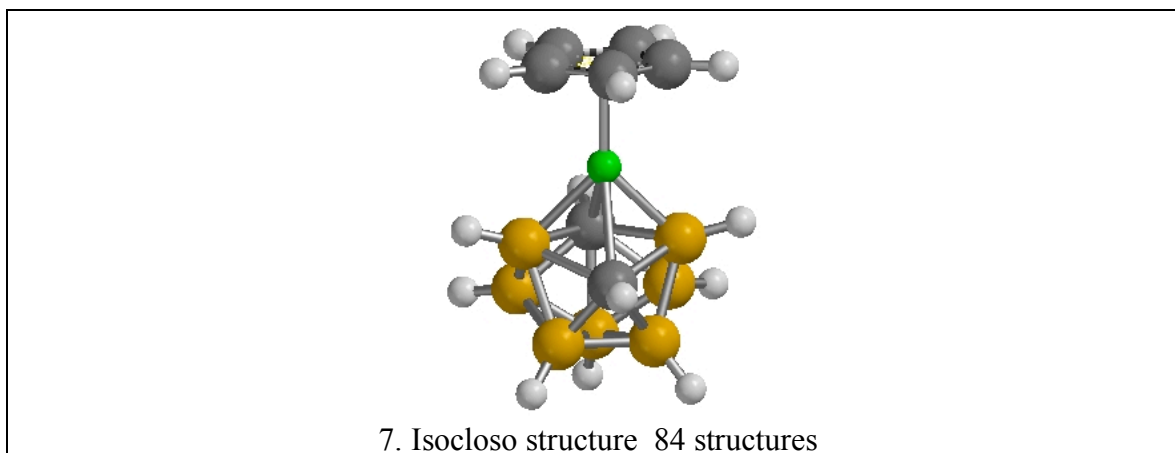
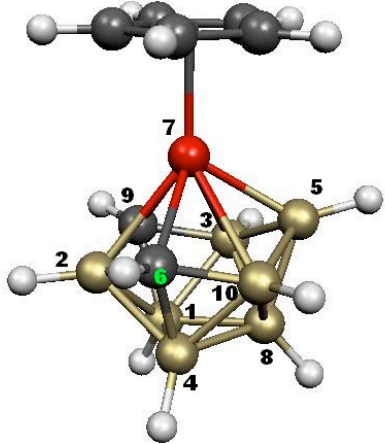
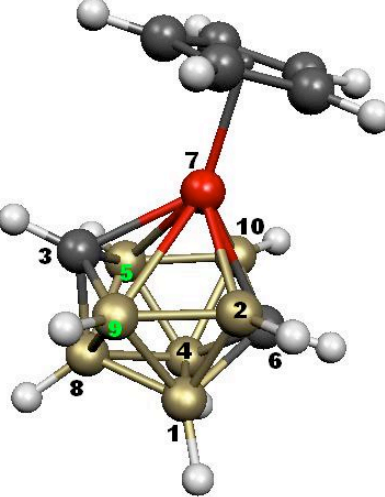
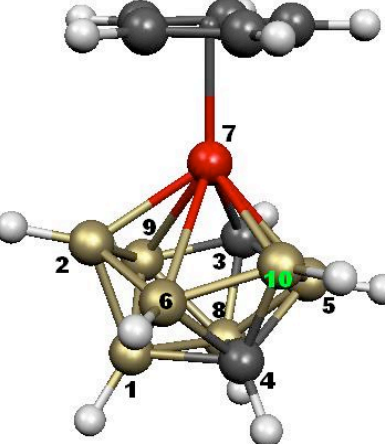


Table 2. Distance table for the best structures

 <p>1. -527.57485904 0.0 kcal/mole Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.852834</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.801111</td><td>2.764054</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.795200</td><td>1.852799</td><td>2.875191</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.958684</td><td>3.365044</td><td>1.779896</td><td>2.958673</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.758768</td><td>1.629902</td><td>3.189999</td><td>1.658585</td><td>2.844047</td></tr> <tr><td>7 Re</td><td>3.119608</td><td>2.380669</td><td>2.395379</td><td>3.119596</td><td>2.092600</td></tr> <tr><td>8 B</td><td>1.801814</td><td>2.897319</td><td>1.809762</td><td>1.801727</td><td>1.815278</td></tr> <tr><td>9 C</td><td>1.658558</td><td>1.629935</td><td>1.612970</td><td>2.758712</td><td>2.843991</td></tr> <tr><td>10 B</td><td>2.875197</td><td>2.763989</td><td>2.797900</td><td>1.801083</td><td>1.779924</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Re</td><td>2.082067</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.744453</td><td>3.082703</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>2.707100</td><td>2.082037</td><td>2.744473</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.612965</td><td>2.395356</td><td>1.809666</td><td>3.189925</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.852834	0.000000				3 B	1.801111	2.764054	0.000000			4 B	1.795200	1.852799	2.875191	0.000000		5 B	2.958684	3.365044	1.779896	2.958673	0.000000	6 C	2.758768	1.629902	3.189999	1.658585	2.844047	7 Re	3.119608	2.380669	2.395379	3.119596	2.092600	8 B	1.801814	2.897319	1.809762	1.801727	1.815278	9 C	1.658558	1.629935	1.612970	2.758712	2.843991	10 B	2.875197	2.763989	2.797900	1.801083	1.779924		6	7	8	9	10	6 C	0.000000					7 Re	2.082067	0.000000				8 B	2.744453	3.082703	0.000000			9 C	2.707100	2.082037	2.744473	0.000000		10 B	1.612965	2.395356	1.809666	3.189925	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.852834	0.000000																																																																																																					
3 B	1.801111	2.764054	0.000000																																																																																																				
4 B	1.795200	1.852799	2.875191	0.000000																																																																																																			
5 B	2.958684	3.365044	1.779896	2.958673	0.000000																																																																																																		
6 C	2.758768	1.629902	3.189999	1.658585	2.844047																																																																																																		
7 Re	3.119608	2.380669	2.395379	3.119596	2.092600																																																																																																		
8 B	1.801814	2.897319	1.809762	1.801727	1.815278																																																																																																		
9 C	1.658558	1.629935	1.612970	2.758712	2.843991																																																																																																		
10 B	2.875197	2.763989	2.797900	1.801083	1.779924																																																																																																		
	6	7	8	9	10																																																																																																		
6 C	0.000000																																																																																																						
7 Re	2.082067	0.000000																																																																																																					
8 B	2.744453	3.082703	0.000000																																																																																																				
9 C	2.707100	2.082037	2.744473	0.000000																																																																																																			
10 B	1.612965	2.395356	1.809666	3.189925	0.000000																																																																																																		
 <p>2. -527.56846565 +4.0 Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.802470</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.724124</td><td>2.842412</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.793200</td><td>2.911555</td><td>2.724124</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.875312</td><td>3.350409</td><td>1.626344</td><td>1.812114</td><td>0.000000</td></tr> <tr><td>6 C</td><td>1.703124</td><td>1.666550</td><td>3.037479</td><td>1.703124</td><td>2.649712</td></tr> <tr><td>7 Re</td><td>3.086721</td><td>2.101999</td><td>2.084936</td><td>3.086721</td><td>2.389531</td></tr> <tr><td>8 B</td><td>1.786999</td><td>2.946752</td><td>1.644188</td><td>1.786999</td><td>1.832610</td></tr> <tr><td>9 B</td><td>1.812126</td><td>1.767103</td><td>1.626320</td><td>2.875319</td><td>2.779200</td></tr> <tr><td>10 B</td><td>2.911566</td><td>2.915600</td><td>2.842497</td><td>1.802489</td><td>1.767071</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Re</td><td>2.314219</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.730129</td><td>3.117848</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.649798</td><td>2.389638</td><td>1.832535</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.666515</td><td>2.102041</td><td>2.946816</td><td>3.350526</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.802470	0.000000				3 C	2.724124	2.842412	0.000000			4 B	1.793200	2.911555	2.724124	0.000000		5 B	2.875312	3.350409	1.626344	1.812114	0.000000	6 C	1.703124	1.666550	3.037479	1.703124	2.649712	7 Re	3.086721	2.101999	2.084936	3.086721	2.389531	8 B	1.786999	2.946752	1.644188	1.786999	1.832610	9 B	1.812126	1.767103	1.626320	2.875319	2.779200	10 B	2.911566	2.915600	2.842497	1.802489	1.767071		6	7	8	9	10	6 C	0.000000					7 Re	2.314219	0.000000				8 B	2.730129	3.117848	0.000000			9 B	2.649798	2.389638	1.832535	0.000000		10 B	1.666515	2.102041	2.946816	3.350526	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.802470	0.000000																																																																																																					
3 C	2.724124	2.842412	0.000000																																																																																																				
4 B	1.793200	2.911555	2.724124	0.000000																																																																																																			
5 B	2.875312	3.350409	1.626344	1.812114	0.000000																																																																																																		
6 C	1.703124	1.666550	3.037479	1.703124	2.649712																																																																																																		
7 Re	3.086721	2.101999	2.084936	3.086721	2.389531																																																																																																		
8 B	1.786999	2.946752	1.644188	1.786999	1.832610																																																																																																		
9 B	1.812126	1.767103	1.626320	2.875319	2.779200																																																																																																		
10 B	2.911566	2.915600	2.842497	1.802489	1.767071																																																																																																		
	6	7	8	9	10																																																																																																		
6 C	0.000000																																																																																																						
7 Re	2.314219	0.000000																																																																																																					
8 B	2.730129	3.117848	0.000000																																																																																																				
9 B	2.649798	2.389638	1.832535	0.000000																																																																																																			
10 B	1.666515	2.102041	2.946816	3.350526	0.000000																																																																																																		
 <p>3. -527.55909109 +9.9</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.794728</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.753671</td><td>2.856699</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.728420</td><td>2.805983</td><td>2.618285</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.879475</td><td>3.342115</td><td>1.608330</td><td>1.741046</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.768723</td><td>1.740973</td><td>3.185577</td><td>1.699844</td><td>2.755674</td></tr> <tr><td>7 Re</td><td>3.085137</td><td>2.111049</td><td>2.094605</td><td>2.947996</td><td>2.362681</td></tr> <tr><td>8 B</td><td>1.795615</td><td>2.936076</td><td>1.652271</td><td>1.702552</td><td>1.818896</td></tr> <tr><td>9 B</td><td>1.820820</td><td>1.775896</td><td>1.617859</td><td>2.740310</td><td>2.740723</td></tr> <tr><td>10 B</td><td>2.930150</td><td>2.954030</td><td>2.852576</td><td>1.746655</td><td>1.757197</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 Re</td><td>2.396504</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.834466</td><td>3.105206</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.770168</td><td>2.395696</td><td>1.805838</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.739378</td><td>2.098617</td><td>2.937152</td><td>3.356115</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.794728	0.000000				3 C	2.753671	2.856699	0.000000			4 C	1.728420	2.805983	2.618285	0.000000		5 B	2.879475	3.342115	1.608330	1.741046	0.000000	6 B	1.768723	1.740973	3.185577	1.699844	2.755674	7 Re	3.085137	2.111049	2.094605	2.947996	2.362681	8 B	1.795615	2.936076	1.652271	1.702552	1.818896	9 B	1.820820	1.775896	1.617859	2.740310	2.740723	10 B	2.930150	2.954030	2.852576	1.746655	1.757197		6	7	8	9	10	6 B	0.000000					7 Re	2.396504	0.000000				8 B	2.834466	3.105206	0.000000			9 B	2.770168	2.395696	1.805838	0.000000		10 B	1.739378	2.098617	2.937152	3.356115	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.794728	0.000000																																																																																																					
3 C	2.753671	2.856699	0.000000																																																																																																				
4 C	1.728420	2.805983	2.618285	0.000000																																																																																																			
5 B	2.879475	3.342115	1.608330	1.741046	0.000000																																																																																																		
6 B	1.768723	1.740973	3.185577	1.699844	2.755674																																																																																																		
7 Re	3.085137	2.111049	2.094605	2.947996	2.362681																																																																																																		
8 B	1.795615	2.936076	1.652271	1.702552	1.818896																																																																																																		
9 B	1.820820	1.775896	1.617859	2.740310	2.740723																																																																																																		
10 B	2.930150	2.954030	2.852576	1.746655	1.757197																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Re	2.396504	0.000000																																																																																																					
8 B	2.834466	3.105206	0.000000																																																																																																				
9 B	2.770168	2.395696	1.805838	0.000000																																																																																																			
10 B	1.739378	2.098617	2.937152	3.356115	0.000000																																																																																																		

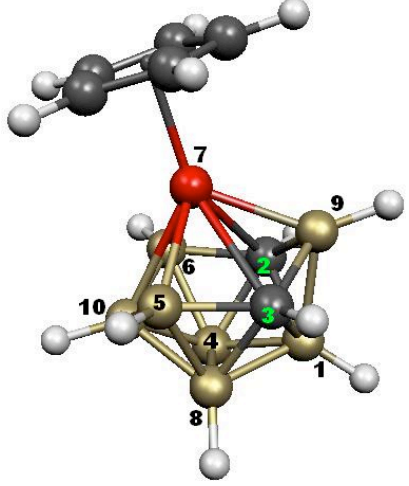
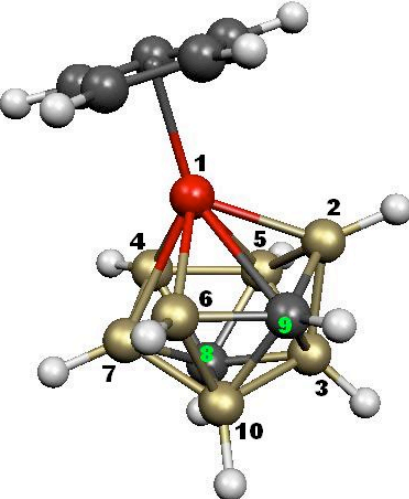
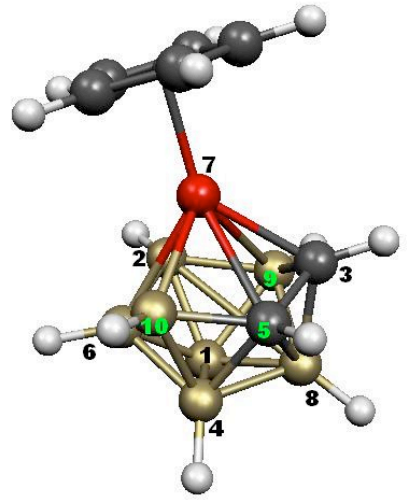
 <p>4. -527.55209769 +14.3 Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 C</td><td>1.699089</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>1.699089</td><td>2.509200</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.771305</td><td>1.733385</td><td>2.736249</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.872601</td><td>3.195742</td><td>1.676492</td><td>2.904241</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.872601</td><td>1.676492</td><td>3.195742</td><td>1.778971</td><td>2.950000</td></tr> <tr><td>7 Re</td><td>3.082573</td><td>2.315919</td><td>2.315919</td><td>3.098233</td><td>2.113253</td></tr> <tr><td>8 B</td><td>1.771305</td><td>2.736249</td><td>1.733385</td><td>1.786400</td><td>1.778971</td></tr> <tr><td>9 B</td><td>1.813052</td><td>1.666050</td><td>1.666050</td><td>2.920336</td><td>2.915545</td></tr> <tr><td>10 B</td><td>2.840056</td><td>2.667336</td><td>2.667336</td><td>1.795520</td><td>1.751542</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 Re</td><td>2.113253</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.904241</td><td>3.098233</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.915545</td><td>2.089558</td><td>2.920336</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.751542</td><td>2.413717</td><td>1.795520</td><td>3.342245</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.699089	0.000000				3 C	1.699089	2.509200	0.000000			4 B	1.771305	1.733385	2.736249	0.000000		5 B	2.872601	3.195742	1.676492	2.904241	0.000000	6 B	2.872601	1.676492	3.195742	1.778971	2.950000	7 Re	3.082573	2.315919	2.315919	3.098233	2.113253	8 B	1.771305	2.736249	1.733385	1.786400	1.778971	9 B	1.813052	1.666050	1.666050	2.920336	2.915545	10 B	2.840056	2.667336	2.667336	1.795520	1.751542		6	7	8	9	10	6 B	0.000000					7 Re	2.113253	0.000000				8 B	2.904241	3.098233	0.000000			9 B	2.915545	2.089558	2.920336	0.000000		10 B	1.751542	2.413717	1.795520	3.342245	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 C	1.699089	0.000000																																																																																																					
3 C	1.699089	2.509200	0.000000																																																																																																				
4 B	1.771305	1.733385	2.736249	0.000000																																																																																																			
5 B	2.872601	3.195742	1.676492	2.904241	0.000000																																																																																																		
6 B	2.872601	1.676492	3.195742	1.778971	2.950000																																																																																																		
7 Re	3.082573	2.315919	2.315919	3.098233	2.113253																																																																																																		
8 B	1.771305	2.736249	1.733385	1.786400	1.778971																																																																																																		
9 B	1.813052	1.666050	1.666050	2.920336	2.915545																																																																																																		
10 B	2.840056	2.667336	2.667336	1.795520	1.751542																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Re	2.113253	0.000000																																																																																																					
8 B	2.904241	3.098233	0.000000																																																																																																				
9 B	2.915545	2.089558	2.920336	0.000000																																																																																																			
10 B	1.751542	2.413717	1.795520	3.342245	0.000000																																																																																																		
 <p>5. -527.54724903 +17.3 Cs</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 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.120401</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.077033</td><td>1.778783</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.098366</td><td>2.960887</td><td>2.890134</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.385709</td><td>1.737266</td><td>1.764338</td><td>1.751227</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.120401</td><td>2.927000</td><td>2.907532</td><td>2.960887</td><td>3.341773</td></tr> <tr><td>7 B</td><td>2.385709</td><td>3.341773</td><td>2.853856</td><td>1.751227</td><td>2.784200</td></tr> <tr><td>8 C</td><td>2.950417</td><td>2.803202</td><td>1.706946</td><td>1.721591</td><td>1.733240</td></tr> <tr><td>9 C</td><td>2.330212</td><td>1.670287</td><td>1.707007</td><td>3.202796</td><td>2.631373</td></tr> <tr><td>10 B</td><td>3.077033</td><td>2.907532</td><td>1.807200</td><td>2.890134</td><td>2.853856</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.737266</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.803202</td><td>1.733240</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.670287</td><td>2.631373</td><td>2.597527</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.778783</td><td>1.764338</td><td>1.706946</td><td>1.707007</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 Re	0.000000					2 B	2.120401	0.000000				3 B	3.077033	1.778783	0.000000			4 B	2.098366	2.960887	2.890134	0.000000		5 B	2.385709	1.737266	1.764338	1.751227	0.000000	6 B	2.120401	2.927000	2.907532	2.960887	3.341773	7 B	2.385709	3.341773	2.853856	1.751227	2.784200	8 C	2.950417	2.803202	1.706946	1.721591	1.733240	9 C	2.330212	1.670287	1.707007	3.202796	2.631373	10 B	3.077033	2.907532	1.807200	2.890134	2.853856		6	7	8	9	10	6 B	0.000000					7 B	1.737266	0.000000				8 C	2.803202	1.733240	0.000000			9 C	1.670287	2.631373	2.597527	0.000000		10 B	1.778783	1.764338	1.706946	1.707007	0.000000
	1	2	3	4	5																																																																																																		
1 Re	0.000000																																																																																																						
2 B	2.120401	0.000000																																																																																																					
3 B	3.077033	1.778783	0.000000																																																																																																				
4 B	2.098366	2.960887	2.890134	0.000000																																																																																																			
5 B	2.385709	1.737266	1.764338	1.751227	0.000000																																																																																																		
6 B	2.120401	2.927000	2.907532	2.960887	3.341773																																																																																																		
7 B	2.385709	3.341773	2.853856	1.751227	2.784200																																																																																																		
8 C	2.950417	2.803202	1.706946	1.721591	1.733240																																																																																																		
9 C	2.330212	1.670287	1.707007	3.202796	2.631373																																																																																																		
10 B	3.077033	2.907532	1.807200	2.890134	2.853856																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	1.737266	0.000000																																																																																																					
8 C	2.803202	1.733240	0.000000																																																																																																				
9 C	1.670287	2.631373	2.597527	0.000000																																																																																																			
10 B	1.778783	1.764338	1.706946	1.707007	0.000000																																																																																																		
 <p>6. -527.53894527 +22.54</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.790342</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.758476</td><td>2.844937</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.797892</td><td>2.906156</td><td>2.743549</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>2.757133</td><td>3.212220</td><td>1.547345</td><td>1.742545</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.798796</td><td>1.751527</td><td>3.190336</td><td>1.767290</td><td>2.650818</td></tr> <tr><td>7 Re</td><td>3.104199</td><td>2.115727</td><td>2.069953</td><td>3.101877</td><td>2.311411</td></tr> <tr><td>8 B</td><td>1.778986</td><td>2.925420</td><td>1.686307</td><td>1.786365</td><td>1.756638</td></tr> <tr><td>9 B</td><td>1.829151</td><td>1.775288</td><td>1.617092</td><td>2.869184</td><td>2.629846</td></tr> <tr><td>10 B</td><td>2.926711</td><td>2.941602</td><td>2.809696</td><td>1.797011</td><td>1.684148</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 Re</td><td>2.425965</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.852757</td><td>3.130135</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.795693</td><td>2.385920</td><td>1.807386</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.735396</td><td>2.114258</td><td>2.929384</td><td>3.335902</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.790342	0.000000				3 C	2.758476	2.844937	0.000000			4 B	1.797892	2.906156	2.743549	0.000000		5 C	2.757133	3.212220	1.547345	1.742545	0.000000	6 B	1.798796	1.751527	3.190336	1.767290	2.650818	7 Re	3.104199	2.115727	2.069953	3.101877	2.311411	8 B	1.778986	2.925420	1.686307	1.786365	1.756638	9 B	1.829151	1.775288	1.617092	2.869184	2.629846	10 B	2.926711	2.941602	2.809696	1.797011	1.684148		6	7	8	9	10	6 B	0.000000					7 Re	2.425965	0.000000				8 B	2.852757	3.130135	0.000000			9 B	2.795693	2.385920	1.807386	0.000000		10 B	1.735396	2.114258	2.929384	3.335902	0.000000
	1	2	3	4	5																																																																																																		
1 B	0.000000																																																																																																						
2 B	1.790342	0.000000																																																																																																					
3 C	2.758476	2.844937	0.000000																																																																																																				
4 B	1.797892	2.906156	2.743549	0.000000																																																																																																			
5 C	2.757133	3.212220	1.547345	1.742545	0.000000																																																																																																		
6 B	1.798796	1.751527	3.190336	1.767290	2.650818																																																																																																		
7 Re	3.104199	2.115727	2.069953	3.101877	2.311411																																																																																																		
8 B	1.778986	2.925420	1.686307	1.786365	1.756638																																																																																																		
9 B	1.829151	1.775288	1.617092	2.869184	2.629846																																																																																																		
10 B	2.926711	2.941602	2.809696	1.797011	1.684148																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 Re	2.425965	0.000000																																																																																																					
8 B	2.852757	3.130135	0.000000																																																																																																				
9 B	2.795693	2.385920	1.807386	0.000000																																																																																																			
10 B	1.735396	2.114258	2.929384	3.335902	0.000000																																																																																																		

Table 3. Energy ranking

No	Initial structure	Final energy (a.u.)	D kcal/mole	Remarks
1	1-TetrTriPri1_Re_v6_C2_v35d	-527.57485904	0.00	
2	1-TetrTriPri1_Re_v6_C2_v36b	-527.57485904	0.00	
3	2-TetrTriPri2_Re_v6_C2_v34a	-527.57485904	0.00	
4	4-BicapSqAntipr_Re_v5_C2_u	-527.57485904	0.00	
5	7-Isocloso_Re_v4_C2_m	-527.57485904	0.00	
6	7-Isocloso_Re_v5b_C2_t	-527.57485904	0.00	
7	7-Isocloso_Re_v6_C2_v2_c	-527.57485904	0.00	
8	2-TetrTriPri2_Re_v6_C2_v44b	-527.57468931	0.11	
9	7-Isocloso_Re_v6_C2_v2_r	-527.57468931	0.11	
10	1-TetrTriPri1_Re_v6_C2_v65c	-527.56846565	4.01	
11	2-TetrTriPri2_Re_v6_C2_v35a	-527.56846565	4.01	
12	7-Isocloso_Re_v6_C2_v2_b	-527.56846565	4.01	
13	7-Isocloso_Re_v6_C2_v2_s	-527.56846565	4.01	
14	1-TetrTriPri1_Re_v6_C2_v33	-527.56845773	4.02	
15	7-Isocloso_Re_v4_C2_a	-527.56845773	4.02	
16	4-BicapSqAntipr_Re_v5_C2_s	-527.56844823	4.02	
17	2-TetrTriPri2_Re_v6_C2_v46	-527.56844820	4.02	
18	1-TetrTriPri1_Re_v6_C2_v65d	-527.55909109	9.89	
19	7-Isocloso_Re_v6_C2_v2_e	-527.55909108	9.89	
20	2-TetrTriPri2_Re_v6_C2_v35b	-527.55909105	9.89	
21	2-TetrTriPri2_Re_v6_C2_v44a	-527.55909105	9.89	
22	6-AntiPr-Re_v4_C2_v2_d	-527.55909104	9.89	
23	5-PentagPrism_Re_v3_d	-527.55909103	9.89	
24	2-TetrTriPri2_Re_v6_C2_v45e	-527.55909102	9.89	
25	1-TetrTriPri1_Re_v6_C2_v45a	-527.55909100	9.89	
26	3-BicapCub_Re_v4b_C2_l	-527.55909097	9.89	
27	7-Isocloso_Re_v6_C2_v2_q	-527.55909096	9.89	
28	7-Isocloso_Re_v6_C2_v2_i	-527.55909069	9.89	
29	1-TetrTriPri1_Re_v4_C2_v55c	-527.55909052	9.89	
30	1-TetrTriPri1_Re_v6_C2_v65a	-527.55209769	14.28	
31	2-TetrTriPri2_Re_v6_C2_v66	-527.55209769	14.28	
32	7-Isocloso_Re_v6_C2_v2_u	-527.55209769	14.28	
33	2-TetrTriPri2_Re_v3_C2_v44a	-527.55190505	14.40	
34	7-Isocloso_Re_v6_C2_v2_k	-527.55190505	14.40	
35	2-TetrTriPri2_Re_v6_C2_v55a	-527.55190504	14.40	
36	4-BicapSqAntipr_Re_v5_C2_r	-527.55190504	14.40	
37	7-Isocloso_Re_v5b_C2_f	-527.54724903	17.33	

38	2-TetrTriPri2_Re_v6_C2_v56a	-527.54724902	17.33	
39	7-Isocloso_Re_v4_C2_f	-527.54724902	17.33	
40	2-TetrTriPri2_Re_v6_C2_v54a	-527.54706485	17.44	
41	7-Isocloso_Re_v6_C2_v2_f	-527.54706485	17.44	
42	7-Isocloso_Re_v6_C2_v2_p	-527.54706485	17.44	
43	1-TetrTriPri1_Re_v6_C2_v66	-527.53894527	22.54	C-C
44	2-TetrTriPri2_Re_v6_C2_v54b	-527.53894526	22.54	C-C
45	1-TetrTriPri1_Re_v4_C2_v45b	-527.53894525	22.54	C-C
46	7-Isocloso_Re_v6_C2_v2_d	-527.53894525	22.54	C-C
47	7-Isocloso_Re_v6_C2_v2_j	-527.53894525	22.54	C-C
48	7-Isocloso_Re_v6_C2_v2_t	-527.53894525	22.54	C-C
49	2-TetrTriPri2_Re_v6_C2_v36	-527.53894523	22.54	C-C
50	2-TetrTriPri2_Re_v6_C2_v45d	-527.53894519	22.54	C-C
51	1-TetrTriPri1_Re_v4_C2_v34b	-527.53867122	22.71	
52	6-AntiPr-Re_v4_C2_v2_s	-527.53636886	24.15	
53	1-TetrTriPri1_Re_v6_C2_v35b	-527.53568784	24.58	C-C
54	1-TetrTriPri1_Re_v6_C2_v55a	-527.53568784	24.58	C-C
55	2-TetrTriPri2_Re_v6_C2_v34b	-527.53568784	24.58	C-C
56	2-TetrTriPri2_Re_v6_C2_v45c	-527.53568784	24.58	C-C
57	4-BicapSqAntipr_Re_v5_C2_b_r-28	-527.53568784	24.58	C-C
58	5-PentagPrism_Re_v3_c	-527.53568784	24.58	C-C
59	5-PentagPrism_Re_v3_l	-527.53568784	24.58	C-C
60	7-Isocloso_Re_v6_C2_v2_a	-527.53568784	24.58	C-C
61	7-Isocloso_Re_v6_C2_v2_n	-527.53568784	24.58	C-C
62	6-AntiPr-Re_v4_C2_v2_h	-527.53553928	24.67	
63	6-AntiPr-Re_v4_C2_v2_o	-527.53553928	24.67	
64	4-BicapSqAntipr_Re_v5_C2_b_i-28	-527.53528453	24.83	C-C
65	2-TetrTriPri2_Re_v3_C2_v64b	-527.53361518	25.88	
66	2-TetrTriPri2_Re_v4_C2_v46b	-527.53361518	25.88	
67	2-TetrTriPri2_Re_v5_C2_v34b	-527.53141840	27.26	
68	4-BicapSqAntipr_Re_v5_C2_p	-527.53141838	27.26	
69	7-Isocloso_Re_v5b_C2_l	-527.53141838	27.26	
70	7-Isocloso_Re_v4_C2_o	-527.53141837	27.26	
71	7-Isocloso_Re_v5b_C2_k	-527.53141837	27.26	
72	2-TetrTriPri2_Re_v5_C2_v45a	-527.53141836	27.26	
73	3-BicapCub_Re_v4b_C2_f	-527.53141836	27.26	
74	4-BicapSqAntipr_Re_v5_C2_e	-527.53141836	27.26	
75	6-AntiPr-Re_v4_C2_v2_g	-527.53141836	27.26	
76	7-Isocloso_Re_v5a_C2_g	-527.53141836	27.26	
77	7-Isocloso_Re_v5b_C2_g	-527.53141836	27.26	
78	2-TetrTriPri2_Re_v4_C2_v56a	-527.53141835	27.26	

79	3-BicapCub_Re_v4b_C2_x	-527.53141835	27.26	
80	2-TetrTriPri2_Re_v4_C2_v65b	-527.53141834	27.26	
81	3-BicapCub_Re_v4b_C2_b	-527.53141834	27.26	
82	7-Isocloso_Re_v4_C2_l	-527.53141834	27.26	
83	7-Isocloso_Re_v5a_C2_j	-527.53141834	27.26	
84	3-BicapCub_Re_v4b_C2_t	-527.53141831	27.26	
85	2-TetrTriPri2_Re_v3_C2_v46c	-527.53079501	27.65	
86	4-BicapSqAntipr_Re_v5_C2_a	-527.53079501	27.65	
87	2-TetrTriPri2_Re_v5_C2_v64a	-527.53079500	27.65	C-C
88	5-PentagPrism_Re_v3_i	-527.52811459	29.33	
89	2-TetrTriPri2_Re_v5_C2_v66b	-527.52809931	29.34	
90	7-Isocloso_Re_v5a_C2_r	-527.52809931	29.34	
91	2-TetrTriPri2_Re_v4_C2_v44	-527.52808380	29.35	
92	2-TetrTriPri2_Re_v5_C2_v64c	-527.52477816	31.43	
93	3-BicapCub_Re_v4a_C2_d	-527.52477816	31.43	
94	3-BicapCub_Re_v4b_C2_c	-527.52477816	31.43	
95	7-Isocloso_Re_v4_C2_n	-527.52477816	31.43	
96	7-Isocloso_Re_v5a_C2_n	-527.52477816	31.43	
97	7-Isocloso_Re_v5b_C2_o	-527.52477816	31.43	
98	5-PentagPrism_Re_v3_g	-527.52383809	32.02	C-C
99	7-Isocloso_Re_v4_C2_i	-527.52383766	32.02	C-C
100	2-TetrTriPri2_Re_v6_C2_v55b	-527.52383763	32.02	C-C
101	2-TetrTriPri2_Re_v6_C2_v45b	-527.52383762	32.02	C-C
102	7-Isocloso_Re_v6_C2_v2_h	-527.52383760	32.02	C-C
103	7-Isocloso_Re_v6_C2_v2_l	-527.52383760	32.02	C-C
104	7-Isocloso_Re_v6_C2_v2_m	-527.52383760	32.02	C-C
105	2-TetrTriPri2_Re_v6_C2_v56b	-527.52383746	32.02	C-C
106	4-BicapSqAntipr_Re_v5_C2_k	-527.52383746	32.02	C-C
107	5-PentagPrism_Re_v3_p	-527.52231172	32.97	
108	6-AntiPr-Re_v4_C2_v2_i	-527.52231171	32.97	
109	6-AntiPr-Re_v4_C2_v2_e i-23	-527.51995412	34.45	C-C
110	6-AntiPr-Re_v4_C2_v2_e r-23	-527.51992951	34.47	C-C
111	7-Isocloso_Re_v5a_C2_c	-527.51992951	34.47	C-C
112	2-TetrTriPri2_Re_v3_C2_v44b	-527.51975758	34.58	
113	3-BicapCub_Re_v4b_C2_r	-527.51975758	34.58	
114	5-PentagPrism_Re_v3_m	-527.51975757	34.58	
115	6-AntiPr-Re_v4_C2_v2_j	-527.51927077	34.88	
116	6-AntiPr-Re_v4_C2_v2_p	-527.51716526	36.20	
117	3-BicapCub_Re_v4b_C2_d	-527.51716523	36.20	
118	5-PentagPrism_Re_v3_r	-527.51716523	36.20	
119	3-BicapCub_Re_v4a_C2_a	-527.51680816	36.43	

120	1-TetrTriPri1_Re_v4_C2_v36a	-527.51680815	36.43	
121	4-BicapSqAntipr_Re_v5_C2_m	-527.51650821	36.62	C-C
122	7-Isocloso_Re_v4_C2_u	-527.51650821	36.62	C-C
123	7-Isocloso_Re_v6_C2_v2_g	-527.51650821	36.62	C-C
124	7-Isocloso_Re_v6_C2_v2_o	-527.51637829	36.70	C-C
125	6-AntiPr-Re_v4_C2_v2_r	-527.51569911	37.12	
126	1-TetrTriPri1_Re_v4_C2_v55a	-527.51222460	39.30	
127	1-TetrTriPri1_Re_v4_C2_v33	-527.51076213	40.22	
128	5-PentagPrism_Re_v3_k	-527.51076213	40.22	
129	1-TetrTriPri1_Re_v4_C2_v35b	-527.51076212	40.22	
130	7-Isocloso_Re_v4_C2_s	-527.51027881	40.52	
131	7-Isocloso_Re_v5b_C2_u_r-194	-527.51027881	40.52	
132	2-TetrTriPri2_Re_v5_C2_v44a	-527.50996091	40.72	
133	3-BicapCub_Re_v4b_C2_o	-527.50996090	40.72	
134	7-Isocloso_Re_v5a_C2_l	-527.50996089	40.72	
135	2-TetrTriPri2_Re_v3_C2_v55c	-527.50980978	40.82	
136	3-BicapCub_Re_v4b_C2_h	-527.50980978	40.82	
137	4-BicapSqAntipr_Re_v5_C2_f	-527.50945085	41.04	
138	2-TetrTriPri2_Re_v3_C2_v66a_r-93	-527.50900297	41.32	
139	2-TetrTriPri2_Re_v3_C2_v66b_r-93	-527.50900297	41.32	
140	6-AntiPr-Re_v4_C2_v2_c	-527.50890590	41.39	
141	2-TetrTriPri2_Re_v3_C2_v46b	-527.50787454	42.03	C-C
142	2-TetrTriPri2_Re_v3_C2_v64a	-527.50787454	42.03	C-C
143	2-TetrTriPri2_Re_v5_C2_v65b	-527.50273741	45.26	
144	2-TetrTriPri2_Re_v5_C2_v66a	-527.50273741	45.26	
145	4-BicapSqAntipr_Re_v5_C2_h	-527.50273741	45.26	
146	7-Isocloso_Re_v4_C2_h	-527.50273741	45.26	
147	7-Isocloso_Re_v5a_C2_d	-527.50273741	45.26	
148	7-Isocloso_Re_v5a_C2_s	-527.50273741	45.26	
149	5-PentagPrism_Re_v3_s_r-75	-527.50244401	45.44	
150	5-PentagPrism_Re_v3_o	-527.50244399	45.44	
151	7-Isocloso_Re_v5a_C2_p	-527.50221393	45.58	C-C
152	2-TetrTriPri2_Re_v5_C2_v45c	-527.50221392	45.58	C-C
153	2-TetrTriPri2_Re_v3_C2_v66a_i-93	-527.50168014	45.92	
154	2-TetrTriPri2_Re_v3_C2_v66b	-527.50168014	45.92	
155	3-BicapCub_Re_v4b_C2_s	-527.50123675	46.20	
156	2-TetrTriPri2_Re_v4_C2_v66a	-527.50115672	46.25	
157	1-TetrTriPri1_Re_v4_C2_v35d	-527.50098594	46.36	
158	5-PentagPrism_Re_v3_s_i-75	-527.50033374	46.76	
159	1-TetrTriPri1_Re_v4_C2_v55d	-527.49929810	47.41	
160	7-Isocloso_Re_v5b_C2_q_r-28	-527.49919630	47.48	

161	2-TetrTriPri2_Re_v4_C2_v65d	-527.49919629	47.48	
162	2-TetrTriPri2_Re_v5_C2_v45b	-527.49919629	47.48	
163	4-BicapSqAntipr_Re_v5_C2_c	-527.49919629	47.48	
164	7-Isocloso_Re_v4_C2_c	-527.49919629	47.48	
165	7-Isocloso_Re_v5a_C2_o	-527.49919629	47.48	
166	7-Isocloso_Re_v5b_C2_q_r-181	-527.49919629	47.48	
167	7-Isocloso_Re_v5b_C2_i	-527.49914308	47.51	C-C
168	3-BicapCub_Re_v4b_C2_g	-527.49914306	47.51	C-C
169	5-PentagPrism_Re_v3_t_r-266	-527.49859979	47.85	
170	2-TetrTriPri2_Re_v3_C2_v54b	-527.49710328	48.79	C-C
171	2-TetrTriPri2_Re_v3_C2_v54c	-527.49710328	48.79	C-C
172	1-TetrTriPri1_Re_v4_C2_v44	-527.49673565	49.02	
173	4-BicapSqAntipr_Re_v4_C2_i	-527.49649144	49.18	
174	7-Isocloso_Re_v4_C2_r_r-37	-527.49641301	49.22	
175	1-TetrTriPri1_Re_v4_C2_v45d	-527.49568785	49.68	
176	6-AntiPr-Re_v4_C2_v2_n	-527.49556829	49.75	
177	7-Isocloso_Re_v4_C2_r_i-37	-527.49544774	49.83	
178	1-TetrTriPri1_Re_v4_C2_v45c	-527.49474567	50.27	
179	1-TetrTriPri1_Re_v4_C2_v36b	-527.49451544	50.42	C-C
180	1-TetrTriPri1_Re_v4_C2_v65b	-527.49451544	50.42	C-C
181	5-PentagPrism_Re_v3_f	-527.49420121	50.61	C-C
182	6-AntiPr-Re_v4_C2_v2_l	-527.49420120	50.61	C-C
183	3-BicapCub_Re_v4b_C2_p	-527.49330005	51.18	C-C
184	7-Isocloso_Re_v5b_C2_u_i-194	-527.49145531	52.34	
185	4-BicapSqAntipr_Re_v5_C2_i_r-12	-527.49097355	52.64	C-C
186	7-Isocloso_Re_v5a_C2_q	-527.49097355	52.64	C-C
187	2-TetrTriPri2_Re_v3_C2_v46a	-527.49097354	52.64	C-C
188	2-TetrTriPri2_Re_v3_C2_v46a_r-12	-527.49097354	52.64	C-C
189	2-TetrTriPri2_Re_v3_C2v46ar-12-12	-527.49097354	52.64	C-C
190	2-TetrTriPri2_Re_v5_C2_v64d_i-12	-527.49097354	52.64	C-C
191	2-TetrTriPri2_Re_v5_C2_v64d_r-12	-527.49097354	52.64	C-C
192	2-TetrTriPri2_Re_v5_C2_v65c_i-12	-527.49097354	52.64	C-C
193	2-TetrTriPri2_Re_v5_C2_v65c_r-12	-527.49097354	52.64	C-C
194	4-BicapSqAntipr_Re_v5_C2_i-12	-527.49097354	52.64	C-C
195	4-BicapSqAntipr_Re_v5_C2_i_r-12	-527.49097354	52.64	C-C
196	7-Isocloso_Re_v5a_C2_q_r-12	-527.49097354	52.64	C-C
197	7-Isocloso_Re_v5a_C2_t_i-12	-527.49097354	52.64	C-C
198	7-Isocloso_Re_v5a_C2_t_r-12	-527.49097354	52.64	C-C
199	7-Isocloso_Re_v5b_C2_h	-527.49070663	52.81	
200	7-Isocloso_Re_v4_C2_e	-527.49070662	52.81	
201	2-TetrTriPri2_Re_v5_C2_v35	-527.49070661	52.81	

202	3-BicapCub_Re_v4b_C2_w	-527.49070661	52.81	
203	4-BicapSqAntipr_Re_v5_C2_n	-527.49070661	52.81	
204	7-Isocloso_Re_v5a_C2_i	-527.49070661	52.81	
205	3-BicapCub_Re_v4b_C2_v	-527.49070660	52.81	
206	4-BicapSqAntipr_Re_v5_C2_o	-527.49070660	52.81	
207	2-TetrTriPri2_Re_v6_C2_v55c	-527.49018030	53.14	
208	2-TetrTriPri2_Re_v4_C2_v34	-527.49017005	53.14	
209	1-TetrTriPri1_Re_v4_C2_v35c	-527.48931438	53.68	C-C
210	5-PentagPrism_Re_v3_a	-527.48900875	53.87	
211	3-BicapCub_Re_v4b_C2_i	-527.48796950	54.52	
212	7-Isocloso_Re_v5b_C2_s	-527.48796948	54.52	
213	2-TetrTriPri2_Re_v4_C2_v45b	-527.48774784	54.66	
214	4-BicapSqAntipr_Re_v5_C2_j	-527.48774784	54.66	
215	7-Isocloso_Re_v5a_C2_e	-527.48762121	54.74	
216	2-TetrTriPri2_Re_v5_C2_v65a	-527.48762120	54.74	
217	7-Isocloso_Re_v5b_C2_d	-527.48762120	54.74	
218	7-Isocloso_Re_v5b_C2_p	-527.48762120	54.74	
219	6-AntiPr-Re_v4_C2_v2_q	-527.48562476	55.99	C-C
220	5-PentagPrism_Re_v3_e	-527.48562474	55.99	C-C
221	7-Isocloso_Re_v5a_C2_b_r-15	-527.48537381	56.15	
222	7-Isocloso_Re_v5b_C2_b_r-15	-527.48537381	56.15	
223	7-Isocloso_Re_v5a_C2_b_i-15	-527.48531937	56.19	
224	7-Isocloso_Re_v5b_C2_b_i-15	-527.48531937	56.19	
225	2-TetrTriPri2_Re_v5_C2_v46a	-527.48449534	56.70	C-C
226	4-BicapSqAntipr_Re_v5_C2_l	-527.48449534	56.70	C-C
227	7-Isocloso_Re_v4_C2_t	-527.48449534	56.70	C-C
228	7-Isocloso_Re_v5a_C2_h	-527.48449534	56.70	C-C
229	7-Isocloso_Re_v5a_C2_k	-527.48449534	56.70	C-C
230	2-TetrTriPri2_Re_v5_C2_v36	-527.48449533	56.70	C-C
231	4-BicapSqAntipr_Re_v5_C2_g	-527.48449533	56.70	C-C
232	3-BicapCub_Re_v4b_C2_j	-527.48445563	56.73	C-C
233	6-AntiPr-Re_v4_C2_v2_f	-527.48445563	56.73	C-C
234	2-TetrTriPri2_Re_v4_C2_v54a	-527.48432387	56.81	C-C
235	3-BicapCub_Re_v4b_C2_q	-527.48432387	56.81	C-C
236	1-TetrTriPri1_Re_v6_C2_v45b	-527.48432386	56.81	C-C
237	2-TetrTriPri2_Re_v3_C2_v55a	-527.48366128	57.23	
238	2-TetrTriPri2_Re_v3_C2_v65a	-527.48366128	57.23	
239	5-PentagPrism_Re_v3_j	-527.48338370	57.40	
240	2-TetrTriPri2_Re_v4_C2_v66b_r-11	-527.48332028	57.44	
241	2-TetrTriPri2_Re_v5_C2_v44b	-527.48332028	57.44	
242	4-BicapSqAntipr_Re_v4_C2_b	-527.48332028	57.44	

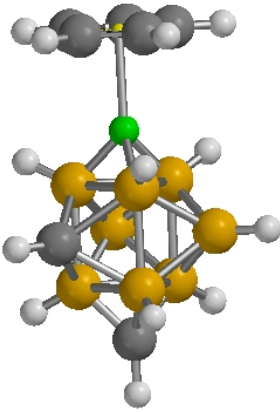
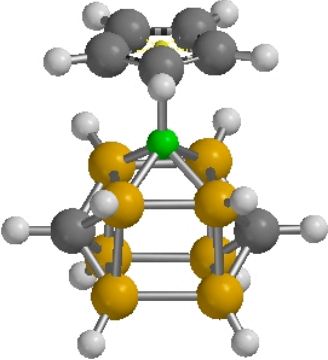
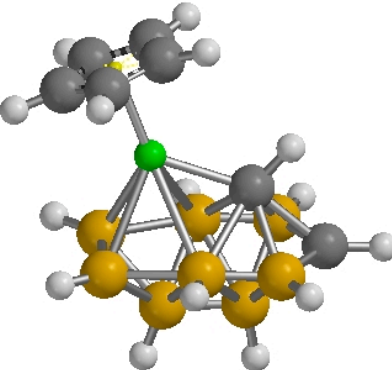
243	7-Isocloso_Re_v5a_C2_m	-527.48332028	57.44	
244	2-TetrTriPri2_Re_v3_C2_v56b	-527.48309433	57.58	
245	2-TetrTriPri2_Re_v4_C2_v66b i-11	-527.48301801	57.63	
246	1-TetrTriPri1_Re_v4_C2_v34a	-527.48282161	57.75	
247	6-AntiPr-Re_v4_C2_v2_b	-527.48081668	59.01	C-C
248	7-Isocloso_Re_v4_C2_b	-527.47781944	60.89	
249	1-TetrTriPri1_Re_v6_C2_v43	-527.47692477	61.45	
250	1-TetrTriPri1_Re_v6_C2_v55b	-527.47660097	61.66	
251	1-TetrTriPri1_Re_v4_C2_v64	-527.47632302	61.83	C-C
252	1-TetrTriPri1_Re_v6_C2_v65b	-527.47623002	61.89	
253	2-TetrTriPri2_Re_v4_C2_v55a	-527.47614217	61.94	C-C
254	7-Isocloso_Re_v5b_C2_n_r-17	-527.47614216	61.94	C-C
255	7-Isocloso_Re_v4_C2_p	-527.47614215	61.94	C-C
256	7-Isocloso_Re_v5b_C2_n i-17	-527.47594021	62.07	C-C
257	1-TetrTriPri1_Re_v6_C2_v35c	-527.47593904	62.07	
258	2-TetrTriPri2_Re_v3_C2_v55b_r-20	-527.47577157	62.18	
259	5-PentagPrism_Re_v3_q	-527.47561366	62.28	C-C
260	2-TetrTriPri2_Re_v3_C2_v55b i-20	-527.47532912	62.46	
261	1-TetrTriPri1_Re_v6_C2_v35a	-527.47446008	63.00	C-C
262	2-TetrTriPri2_Re_v4_C2_v46a	-527.47406685	63.25	C-C
263	7-Isocloso_Re_v5b_C2_e	-527.47404688	63.26	
264	7-Isocloso_Re_v5b_C2_j	-527.47272648	64.09	C-C
265	2-TetrTriPri2_Re_v3_C2_v54a	-527.47217303	64.44	
266	2-TetrTriPri2_Re_v3_C2_v54d	-527.47217303	64.44	
267	2-TetrTriPri2_Re_v5_C2_v64b	-527.47149953	64.86	C-C
268	3-BicapCub_Re_v4b_C2_e	-527.47149953	64.86	C-C
269	2-TetrTriPri2_Re_v4_C2_v45a	-527.47149952	64.86	C-C
270	2-TetrTriPri2_Re_v4_C2_v65c	-527.47149952	64.86	C-C
271	7-Isocloso_Re_v4_C2_q	-527.47149952	64.86	C-C
272	4-BicapSqAntipr_Re_v5_C2_d	-527.47149951	64.86	C-C
273	7-Isocloso_Re_v4_C2_g	-527.47149951	64.86	C-C
274	7-Isocloso_Re_v5b_C2_m	-527.47149951	64.86	C-C
275	7-Isocloso_Re_v5b_C2_c	-527.47149950	64.86	C-C
276	1-TetrTriPri1_Re_v4_C2_v45a	-527.46998512	65.81	C-C
277	2-TetrTriPri2_Re_v4_C2_v35b	-527.46995866	65.82	
278	1-TetrTriPri1_Re_v6_C2_v36a	-527.46994179	65.84	C-C
279	1-TetrTriPri1_Re_v6_C2_v46	-527.46916797	66.32	C-C
280	3-BicapCub_Re_v4b_C2_n	-527.46874086	66.59	C-C
281	7-Isocloso_Re_v4_C2_j	-527.46874086	66.59	C-C
282	2-TetrTriPri2_Re_v5_C2_v34a_r-62	-527.46874085	66.59	C-C
283	7-Isocloso_Re_v5a_C2_f_i-62	-527.46874085	66.59	C-C

284	2-TetrTriPri2_Re_v5_C2_v34a i-62	-527.46845088	66.77	C-C
285	7-Isocloso_Re_v5a_C2_f i-62	-527.46845088	66.77	C-C
286	3-BicapCub_Re_v4a_C2_f	-527.46711047	67.61	
287	4-BicapSqAntipr_Re_v4_C2_h_r-56	-527.46711046	67.61	
288	1-TetrTriPri1_Re_v4_C2_v65a	-527.46626224	68.14	
289	2-TetrTriPri2_Re_v3_C2_v56c	-527.46601666	68.30	C-C
290	4-BicapSqAntipr_Re_v4_C2_h i-56	-527.46457562	69.20	
291	7-Isocloso_Re_v5b_C2_r	-527.46391949	69.61	C-C
292	3-BicapCub_Re_v4a_C2_h_r-130	-527.46346879	69.90	
293	3-BicapCub_Re_v4b_C2_k	-527.46346877	69.90	
294	5-PentagPrism_Re_v3_t i-266	-527.45983754	72.18	
295	2-TetrTriPri2_Re_v4_C2_v36b	-527.45924333	72.55	C-C
296	7-Isocloso_Re_v5a_C2_a_r-303	-527.45806949	73.29	C-C
297	2-TetrTriPri2_Re_v5_C2_v63_r-303	-527.45806944	73.29	C-C
298	6-AntiPr-Re_v4_C2_v2_m	-527.45806944	73.29	C-C
299	7-Isocloso_Re_v5b_C2_a_r-303	-527.45806944	73.29	C-C
300	4-BicapSqAntipr_Re_v5_C2_q	-527.45806943	73.29	C-C
301	2-TetrTriPri2_Re_v4_C2_v35ar-349	-527.45605224	74.55	
302	3-BicapCub_Re_v4a_C2_b	-527.45544243	74.93	
303	4-BicapSqAntipr_Re_v4_C2_c_r-24	-527.45544243	74.93	
304	4-BicapSqAntipr_Re_v5_C2_t	-527.45540154	74.96	
305	2-TetrTriPri2_Re_v5_C2_v55_r-36	-527.45540152	74.96	C-C
306	7-Isocloso_Re_v5a_C2_u_r-36	-527.45540152	74.96	C-C
307	6-AntiPr-Re_v4_C2_v2_k	-527.45373603	76.00	C-C
308	6-AntiPr-Re_v4_C2_v2_t	-527.45373602	76.00	C-C
309	6-AntiPr-Re_v4_C2_v2_a	-527.45286023	76.55	C-C
310	2-TetrTriPri2_Re_v3_C2_v65b	-527.45270420	76.65	C-C
311	2-TetrTriPri2_Re_v4_C2_v64a	-527.45233733	76.88	C-C
312	2-TetrTriPri2_Re_v4_C2_v36a_r-86	-527.45233728	76.88	C-C
313	7-Isocloso_Re_v4_C2_k	-527.45233728	76.88	C-C
314	3-BicapCub_Re_v4b_C2_a	-527.45177788	77.23	C-C
315	2-TetrTriPri2_Re_v3_C2_v45a	-527.44894530	79.01	
316	3-BicapCub_Re_v4a_C2_g	-527.44759704	79.86	C-C
317	2-TetrTriPri2_Re_v4_C2_v65a_r-108	-527.44615473	80.76	C-C
318	5-PentagPrism_Re_v3_n_r-61	-527.44550469	81.17	C-C
319	2-TetrTriPri2_Re_v4_C2_v36a	-527.44474247	81.65	C-C
320	3-BicapCub_Re_v4b_C2_u	-527.44453613	81.78	
321	1-TetrTriPri1_Re_v6_C2_v55c	-527.44443012	81.84	C-C
322	4-BicapSqAntipr_Re_v4_C2_k	-527.44385923	82.20	C-C
323	4-BicapSqAntipr_Re_v4_C2_l	-527.44385923	82.20	
324	2-TetrTriPri2_Re_v5_C2_v63 r-303	-527.44343913	82.47	C-C

325	7-Isocloso_Re_v5a_C2_a i-303	-527.44343913	82.47	C-C
326	7-Isocloso_Re_v5b_C2_a i-303	-527.44343912	82.47	C-C
327	5-PentagPrism_Re_v3_n i-61	-527.44216026	83.27	C-C
328	4-BicapSqAntipr_Re_v4_C2_f	-527.44076670	84.14	
329	4-BicapSqAntipr_Re_v4_C2_g	-527.44076656	84.14	
330	3-BicapCub_Re_v4a_C2_e	-527.44040666	84.37	
331	1-TetrTriPri1_Re_v6_C2_v55d	-527.43976250	84.77	C-C
332	4-BicapSqAntipr_Re_v4_C2_j	-527.43830193	85.69	
333	4-BicapSqAntipr_Re_v4_C2_m	-527.43830193	85.69	
334	7-Isocloso_Re_v5a_C2_u i-36	-527.43801803	85.87	C-C
335	2-TetrTriPri2_Re_v5_C2_v55 i-36	-527.43801802	85.87	C-C
336	3-BicapCub_Re_v4a_C2_i	-527.43725039	86.35	
337	2-TetrTriPri2_Re_v4_C2_v65a i-108	-527.43642225	86.87	C-C
338	7-Isocloso_Re_v5b_C2_q i	-527.43473441	87.93	
339	3-BicapCub_Re_v4a_C2_h i-130	-527.43244183	89.37	
340	3-BicapCub_Re_v4b_C2_m	-527.42927196	91.36	C-C
341	1-TetrTriPri1_Re_v4_C2_v55b	-527.42897501	91.54	C-C
342	1-TetrTriPri1_Re_v4_C2_v35a	-527.42715930	92.68	C-C
343	4-BicapSqAntipr_Re_v4_C2_c i-24	-527.42490816	94.09	
344	4-BicapSqAntipr_Re_v4_C2_e	-527.42297005	95.31	C-C
345	4-BicapSqAntipr_Re_v4_C2_d	-527.42297004	95.31	C-C
346	3-BicapCub_Re_v4a_C2_c	-527.41750145	98.74	C-C
347	4-BicapSqAntipr_Re_v4_C2_a	-527.41163977	102.42	C-C
348	5-PentagPrism_Re_v3_h	-527.40286744	107.92	C-C
349	2-TetrTriPri2_Re_v4_C2_v35a i-349	-527.39289720	114.18	
350	5-PentagPrism_Re_v3_b	-527.38645991	118.22	C-C
351	2-TetrTriPri2_Re_v4_C2_v55b	-527.36556430	131.33	

11-vertex $\text{CpMnC}_2\text{B}_8\text{H}_{10}$

Table 1. Initial structures (one example from each family) 389 structures in total

Initial structures
 <p>1. Pentacapped trigonal prism 49 structures</p>
 <p>2. Tricapped cube 94 structures</p>
 <p>3. Octahedron fused to pentagonal bipyramid 108 structures</p>

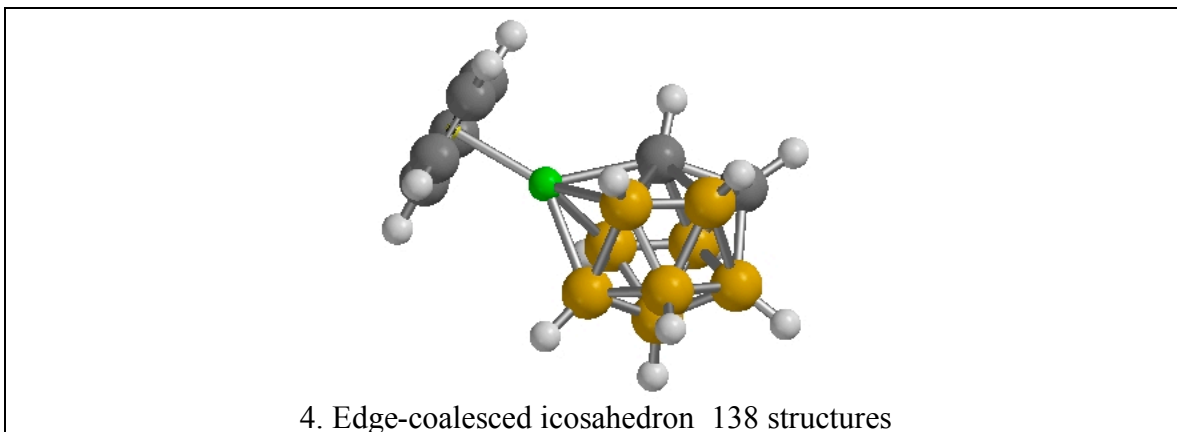
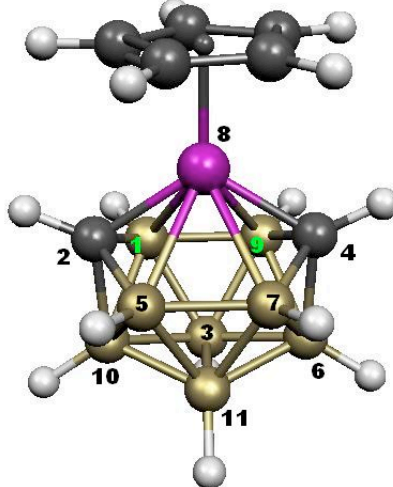
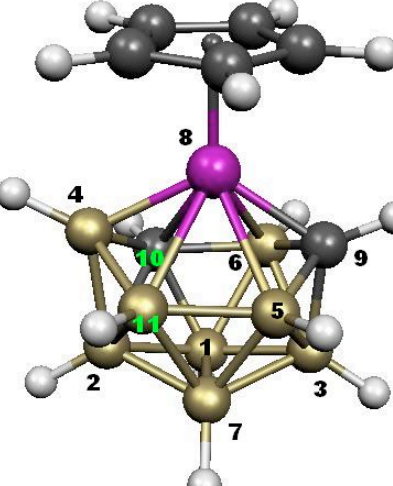
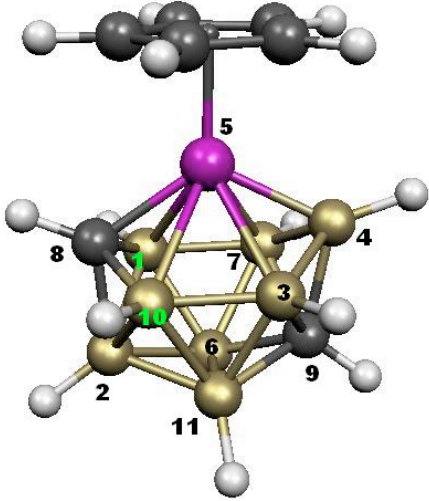
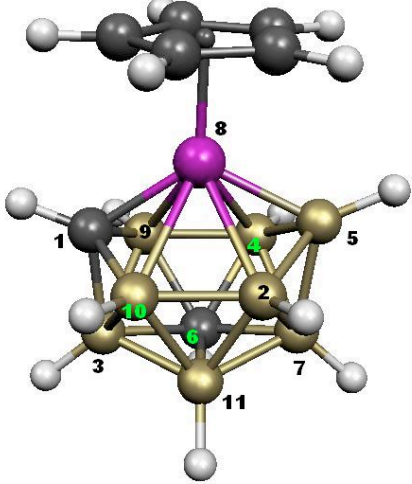
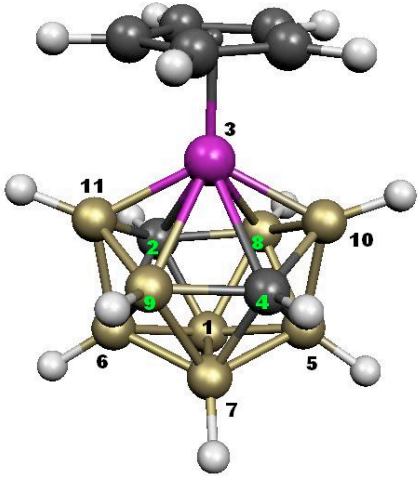
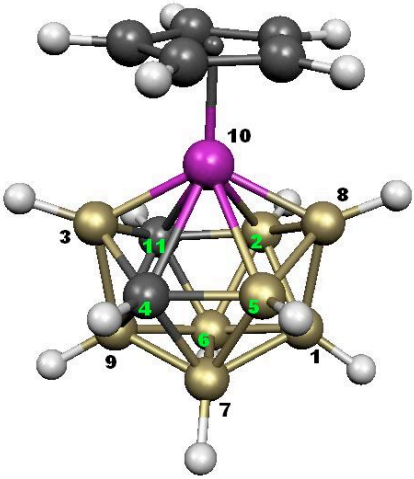
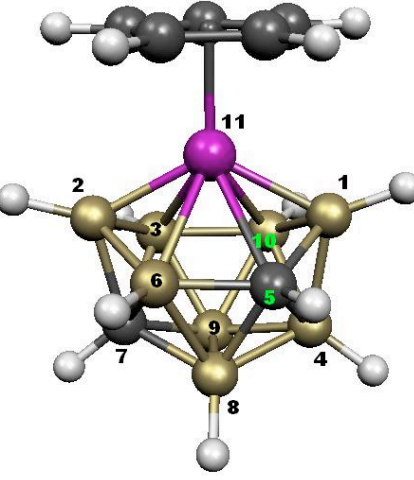
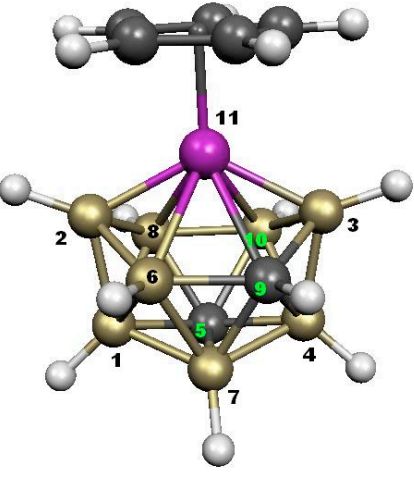
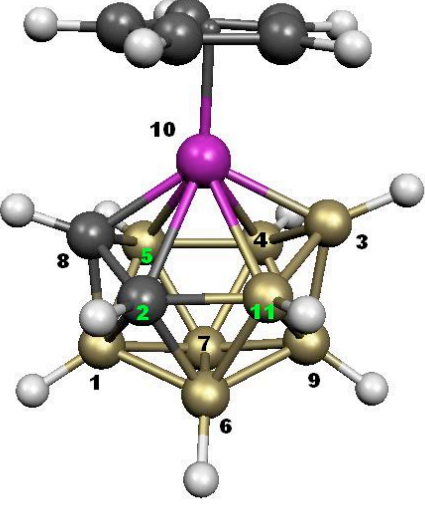
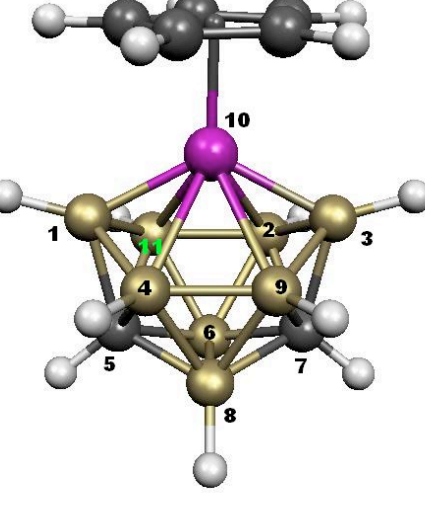


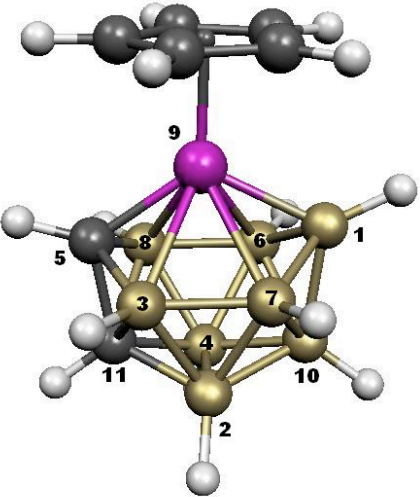
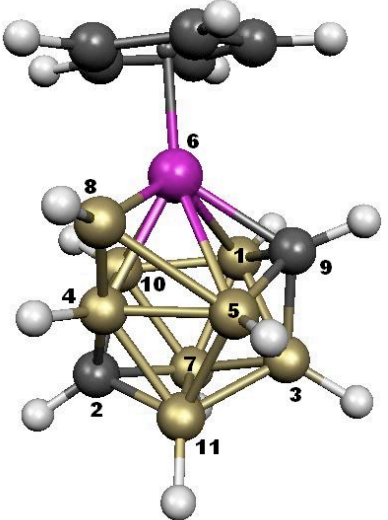
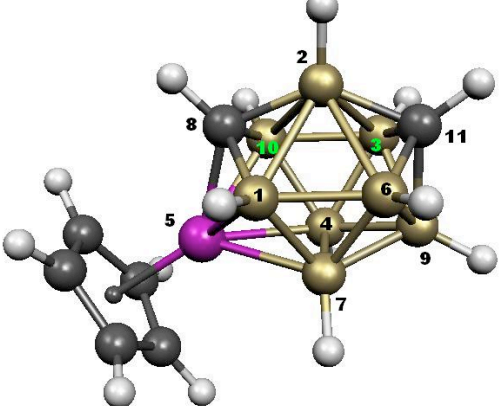
Table 2. Distance table for the best structures

 <p>1. -1625.61945329a.u. Cs(C_{2v}-like) 0.0 kcal/mole</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 C</td><td>1.604162</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.807678</td><td>2.730949</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>2.881232</td><td>3.210218</td><td>2.733234</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.687601</td><td>1.605038</td><td>2.846399</td><td>2.882237</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.947125</td><td>3.489444</td><td>1.774576</td><td>1.638500</td><td>2.947511</td></tr> <tr><td>7 B</td><td>3.227152</td><td>2.884123</td><td>2.846743</td><td>1.605086</td><td>1.786953</td></tr> <tr><td>8 Mn</td><td>2.245386</td><td>1.916639</td><td>3.197650</td><td>1.916473</td><td>2.240251</td></tr> <tr><td>9 B</td><td>1.785855</td><td>2.882937</td><td>1.808054</td><td>1.604225</td><td>3.226962</td></tr> <tr><td>10 B</td><td>1.846854</td><td>1.636052</td><td>1.775732</td><td>3.492582</td><td>1.846572</td></tr> <tr><td>11 B</td><td>2.846800</td><td>2.731398</td><td>1.799400</td><td>2.733621</td><td>1.807325</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>1.844311</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Mn</td><td>3.061409</td><td>2.242608</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.844340</td><td>2.687401</td><td>2.247679</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.961326</td><td>2.950761</td><td>3.061920</td><td>2.950239</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.774942</td><td>1.807858</td><td>3.194999</td><td>2.846907</td><td>1.776076</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.604162	0.000000				3 B	1.807678	2.730949	0.000000			4 C	2.881232	3.210218	2.733234	0.000000		5 B	2.687601	1.605038	2.846399	2.882237	0.000000	6 B	2.947125	3.489444	1.774576	1.638500	2.947511	7 B	3.227152	2.884123	2.846743	1.605086	1.786953	8 Mn	2.245386	1.916639	3.197650	1.916473	2.240251	9 B	1.785855	2.882937	1.808054	1.604225	3.226962	10 B	1.846854	1.636052	1.775732	3.492582	1.846572	11 B	2.846800	2.731398	1.799400	2.733621	1.807325		6	7	8	9	10	6 B	0.000000					7 B	1.844311	0.000000				8 Mn	3.061409	2.242608	0.000000			9 B	1.844340	2.687401	2.247679	0.000000		10 B	2.961326	2.950761	3.061920	2.950239	0.000000	11 B	1.774942	1.807858	3.194999	2.846907	1.776076
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 C	1.604162	0.000000																																																																																																																	
3 B	1.807678	2.730949	0.000000																																																																																																																
4 C	2.881232	3.210218	2.733234	0.000000																																																																																																															
5 B	2.687601	1.605038	2.846399	2.882237	0.000000																																																																																																														
6 B	2.947125	3.489444	1.774576	1.638500	2.947511																																																																																																														
7 B	3.227152	2.884123	2.846743	1.605086	1.786953																																																																																																														
8 Mn	2.245386	1.916639	3.197650	1.916473	2.240251																																																																																																														
9 B	1.785855	2.882937	1.808054	1.604225	3.226962																																																																																																														
10 B	1.846854	1.636052	1.775732	3.492582	1.846572																																																																																																														
11 B	2.846800	2.731398	1.799400	2.733621	1.807325																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.844311	0.000000																																																																																																																	
8 Mn	3.061409	2.242608	0.000000																																																																																																																
9 B	1.844340	2.687401	2.247679	0.000000																																																																																																															
10 B	2.961326	2.950761	3.061920	2.950239	0.000000																																																																																																														
11 B	1.774942	1.807858	3.194999	2.846907	1.776076																																																																																																														
 <p>2. -1625.60777112 +7.3</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.749629</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.771899</td><td>2.936236</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.871221</td><td>1.749619</td><td>3.638482</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.834279</td><td>2.907482</td><td>1.845699</td><td>3.014152</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.832639</td><td>2.906460</td><td>1.856297</td><td>2.946852</td><td>2.686937</td></tr> <tr><td>7 B</td><td>1.783023</td><td>1.756076</td><td>1.786379</td><td>2.898703</td><td>1.797332</td></tr> <tr><td>8 Mn</td><td>3.202826</td><td>3.042741</td><td>3.045385</td><td>1.968582</td><td>2.248879</td></tr> <tr><td>9 C</td><td>2.745262</td><td>3.463495</td><td>1.628701</td><td>3.326382</td><td>1.611428</td></tr> <tr><td>10 C</td><td>1.713865</td><td>1.751845</td><td>2.797771</td><td>1.640401</td><td>3.075466</td></tr> <tr><td>11 B</td><td>2.841864</td><td>1.827603</td><td>2.953590</td><td>1.721893</td><td>1.776316</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.852293</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Mn</td><td>2.198576</td><td>3.204365</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.615720</td><td>2.737448</td><td>1.904678</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>1.666942</td><td>2.707015</td><td>2.173197</td><td>2.763626</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.203782</td><td>1.819341</td><td>2.247291</td><td>2.879328</td><td>2.570011</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.749629	0.000000				3 B	1.771899	2.936236	0.000000			4 B	2.871221	1.749619	3.638482	0.000000		5 B	2.834279	2.907482	1.845699	3.014152	0.000000	6 B	1.832639	2.906460	1.856297	2.946852	2.686937	7 B	1.783023	1.756076	1.786379	2.898703	1.797332	8 Mn	3.202826	3.042741	3.045385	1.968582	2.248879	9 C	2.745262	3.463495	1.628701	3.326382	1.611428	10 C	1.713865	1.751845	2.797771	1.640401	3.075466	11 B	2.841864	1.827603	2.953590	1.721893	1.776316		6	7	8	9	10	6 B	0.000000					7 B	2.852293	0.000000				8 Mn	2.198576	3.204365	0.000000			9 C	1.615720	2.737448	1.904678	0.000000		10 C	1.666942	2.707015	2.173197	2.763626	0.000000	11 B	3.203782	1.819341	2.247291	2.879328	2.570011
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.749629	0.000000																																																																																																																	
3 B	1.771899	2.936236	0.000000																																																																																																																
4 B	2.871221	1.749619	3.638482	0.000000																																																																																																															
5 B	2.834279	2.907482	1.845699	3.014152	0.000000																																																																																																														
6 B	1.832639	2.906460	1.856297	2.946852	2.686937																																																																																																														
7 B	1.783023	1.756076	1.786379	2.898703	1.797332																																																																																																														
8 Mn	3.202826	3.042741	3.045385	1.968582	2.248879																																																																																																														
9 C	2.745262	3.463495	1.628701	3.326382	1.611428																																																																																																														
10 C	1.713865	1.751845	2.797771	1.640401	3.075466																																																																																																														
11 B	2.841864	1.827603	2.953590	1.721893	1.776316																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	2.852293	0.000000																																																																																																																	
8 Mn	2.198576	3.204365	0.000000																																																																																																																
9 C	1.615720	2.737448	1.904678	0.000000																																																																																																															
10 C	1.666942	2.707015	2.173197	2.763626	0.000000																																																																																																														
11 B	3.203782	1.819341	2.247291	2.879328	2.570011																																																																																																														

 <p>3. -1625.60732896 Cs +7.6</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.844819</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.212677</td><td>2.920251</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.026792</td><td>3.661477</td><td>1.723334</td><td>0.000000</td><td></td></tr> <tr><td>5 Mn</td><td>2.250252</td><td>3.061841</td><td>2.217493</td><td>1.957521</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.807290</td><td>1.771886</td><td>2.835745</td><td>2.895224</td><td>3.187759</td></tr> <tr><td>7 B</td><td>1.755308</td><td>2.920213</td><td>2.687000</td><td>1.723346</td><td>2.217263</td></tr> <tr><td>8 C</td><td>1.605965</td><td>1.640330</td><td>2.849095</td><td>3.342741</td><td>1.920522</td></tr> <tr><td>9 C</td><td>2.796359</td><td>2.814422</td><td>1.752018</td><td>1.691403</td><td>2.887198</td></tr> <tr><td>10 B</td><td>2.694500</td><td>1.844889</td><td>1.755208</td><td>3.026687</td><td>2.250426</td></tr> <tr><td>11 B</td><td>2.847311</td><td>1.771888</td><td>1.792699</td><td>2.895180</td><td>3.187857</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>1.792649</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.730427</td><td>2.849087</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.681894</td><td>1.751950</td><td>3.310700</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.847345</td><td>3.212601</td><td>1.606002</td><td>2.796308</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.796600</td><td>2.835638</td><td>2.730428</td><td>1.681848</td><td>1.807312</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.844819	0.000000				3 B	3.212677	2.920251	0.000000			4 B	3.026792	3.661477	1.723334	0.000000		5 Mn	2.250252	3.061841	2.217493	1.957521	0.000000	6 B	1.807290	1.771886	2.835745	2.895224	3.187759	7 B	1.755308	2.920213	2.687000	1.723346	2.217263	8 C	1.605965	1.640330	2.849095	3.342741	1.920522	9 C	2.796359	2.814422	1.752018	1.691403	2.887198	10 B	2.694500	1.844889	1.755208	3.026687	2.250426	11 B	2.847311	1.771888	1.792699	2.895180	3.187857		6	7	8	9	10	6 B	0.000000					7 B	1.792649	0.000000				8 C	2.730427	2.849087	0.000000			9 C	1.681894	1.751950	3.310700	0.000000		10 B	2.847345	3.212601	1.606002	2.796308	0.000000	11 B	1.796600	2.835638	2.730428	1.681848	1.807312
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.844819	0.000000																																																																																																																	
3 B	3.212677	2.920251	0.000000																																																																																																																
4 B	3.026792	3.661477	1.723334	0.000000																																																																																																															
5 Mn	2.250252	3.061841	2.217493	1.957521	0.000000																																																																																																														
6 B	1.807290	1.771886	2.835745	2.895224	3.187759																																																																																																														
7 B	1.755308	2.920213	2.687000	1.723346	2.217263																																																																																																														
8 C	1.605965	1.640330	2.849095	3.342741	1.920522																																																																																																														
9 C	2.796359	2.814422	1.752018	1.691403	2.887198																																																																																																														
10 B	2.694500	1.844889	1.755208	3.026687	2.250426																																																																																																														
11 B	2.847311	1.771888	1.792699	2.895180	3.187857																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.792649	0.000000																																																																																																																	
8 C	2.730427	2.849087	0.000000																																																																																																																
9 C	1.681894	1.751950	3.310700	0.000000																																																																																																															
10 B	2.847345	3.212601	1.606002	2.796308	0.000000																																																																																																														
11 B	1.796600	2.835638	2.730428	1.681848	1.807312																																																																																																														
 <p>4. -1625.60169400 +11.1</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.879195</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.628280</td><td>2.918407</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.870868</td><td>2.681077</td><td>2.914358</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.368295</td><td>1.733632</td><td>3.662995</td><td>1.718599</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.615795</td><td>2.696689</td><td>1.695678</td><td>1.717690</td><td>2.790940</td></tr> <tr><td>7 B</td><td>3.467863</td><td>1.829701</td><td>2.923951</td><td>1.819640</td><td>1.762446</td></tr> <tr><td>8 Mn</td><td>1.917704</td><td>2.240109</td><td>3.036507</td><td>2.226174</td><td>1.975886</td></tr> <tr><td>9 B</td><td>1.598810</td><td>3.206826</td><td>1.840815</td><td>1.759198</td><td>3.017420</td></tr> <tr><td>10 B</td><td>1.614713</td><td>1.773574</td><td>1.831862</td><td>3.216013</td><td>3.043426</td></tr> <tr><td>11 B</td><td>2.737597</td><td>1.783424</td><td>1.771998</td><td>2.833591</td><td>2.908675</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.684477</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Mn</td><td>3.039759</td><td>3.023656</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.738842</td><td>2.914223</td><td>2.214295</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.706175</td><td>2.925413</td><td>2.248605</td><td>2.683014</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.714022</td><td>1.761248</td><td>3.183235</td><td>2.848491</td><td>1.797970</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	2.879195	0.000000				3 B	1.628280	2.918407	0.000000			4 B	2.870868	2.681077	2.914358	0.000000		5 B	3.368295	1.733632	3.662995	1.718599	0.000000	6 C	2.615795	2.696689	1.695678	1.717690	2.790940	7 B	3.467863	1.829701	2.923951	1.819640	1.762446	8 Mn	1.917704	2.240109	3.036507	2.226174	1.975886	9 B	1.598810	3.206826	1.840815	1.759198	3.017420	10 B	1.614713	1.773574	1.831862	3.216013	3.043426	11 B	2.737597	1.783424	1.771998	2.833591	2.908675		6	7	8	9	10	6 C	0.000000					7 B	1.684477	0.000000				8 Mn	3.039759	3.023656	0.000000			9 B	1.738842	2.914223	2.214295	0.000000		10 B	2.706175	2.925413	2.248605	2.683014	0.000000	11 B	1.714022	1.761248	3.183235	2.848491	1.797970
	1	2	3	4	5																																																																																																														
1 C	0.000000																																																																																																																		
2 B	2.879195	0.000000																																																																																																																	
3 B	1.628280	2.918407	0.000000																																																																																																																
4 B	2.870868	2.681077	2.914358	0.000000																																																																																																															
5 B	3.368295	1.733632	3.662995	1.718599	0.000000																																																																																																														
6 C	2.615795	2.696689	1.695678	1.717690	2.790940																																																																																																														
7 B	3.467863	1.829701	2.923951	1.819640	1.762446																																																																																																														
8 Mn	1.917704	2.240109	3.036507	2.226174	1.975886																																																																																																														
9 B	1.598810	3.206826	1.840815	1.759198	3.017420																																																																																																														
10 B	1.614713	1.773574	1.831862	3.216013	3.043426																																																																																																														
11 B	2.737597	1.783424	1.771998	2.833591	2.908675																																																																																																														
	6	7	8	9	10																																																																																																														
6 C	0.000000																																																																																																																		
7 B	1.684477	0.000000																																																																																																																	
8 Mn	3.039759	3.023656	0.000000																																																																																																																
9 B	1.738842	2.914223	2.214295	0.000000																																																																																																															
10 B	2.706175	2.925413	2.248605	2.683014	0.000000																																																																																																														
11 B	1.714022	1.761248	3.183235	2.848491	1.797970																																																																																																														
 <p>5. -1625.59638607 C2-like +14.5</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 C</td><td>1.708443</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Mn</td><td>3.208418</td><td>2.178868</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>2.692516</td><td>2.924226</td><td>2.172859</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.747273</td><td>2.762013</td><td>3.027633</td><td>1.749611</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.762027</td><td>1.747714</td><td>3.026089</td><td>2.760273</td><td>2.908412</td></tr> <tr><td>7 B</td><td>1.768946</td><td>2.692962</td><td>3.204636</td><td>1.706466</td><td>1.762775</td></tr> <tr><td>8 B</td><td>1.839474</td><td>1.669230</td><td>2.207548</td><td>2.565288</td><td>1.837271</td></tr> <tr><td>9 B</td><td>2.850457</td><td>2.566033</td><td>2.203076</td><td>1.672417</td><td>2.917647</td></tr> <tr><td>10 B</td><td>2.904235</td><td>2.900211</td><td>1.955741</td><td>1.639025</td><td>1.741597</td></tr> <tr><td>11 B</td><td>2.876496</td><td>1.638824</td><td>1.955421</td><td>2.902274</td><td>3.611333</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>1.747545</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.912333</td><td>2.848342</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.836213</td><td>1.840822</td><td>3.188523</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.607209</td><td>2.872968</td><td>1.731531</td><td>2.948894</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.708443	0.000000				3 Mn	3.208418	2.178868	0.000000			4 C	2.692516	2.924226	2.172859	0.000000		5 B	1.747273	2.762013	3.027633	1.749611	0.000000	6 B	1.762027	1.747714	3.026089	2.760273	2.908412	7 B	1.768946	2.692962	3.204636	1.706466	1.762775	8 B	1.839474	1.669230	2.207548	2.565288	1.837271	9 B	2.850457	2.566033	2.203076	1.672417	2.917647	10 B	2.904235	2.900211	1.955741	1.639025	1.741597	11 B	2.876496	1.638824	1.955421	2.902274	3.611333		6	7	8	9	10	6 B	0.000000					7 B	1.747545	0.000000				8 B	2.912333	2.848342	0.000000			9 B	1.836213	1.840822	3.188523	0.000000		10 B	3.607209	2.872968	1.731531	2.948894	0.000000						
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 C	1.708443	0.000000																																																																																																																	
3 Mn	3.208418	2.178868	0.000000																																																																																																																
4 C	2.692516	2.924226	2.172859	0.000000																																																																																																															
5 B	1.747273	2.762013	3.027633	1.749611	0.000000																																																																																																														
6 B	1.762027	1.747714	3.026089	2.760273	2.908412																																																																																																														
7 B	1.768946	2.692962	3.204636	1.706466	1.762775																																																																																																														
8 B	1.839474	1.669230	2.207548	2.565288	1.837271																																																																																																														
9 B	2.850457	2.566033	2.203076	1.672417	2.917647																																																																																																														
10 B	2.904235	2.900211	1.955741	1.639025	1.741597																																																																																																														
11 B	2.876496	1.638824	1.955421	2.902274	3.611333																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.747545	0.000000																																																																																																																	
8 B	2.912333	2.848342	0.000000																																																																																																																
9 B	1.836213	1.840822	3.188523	0.000000																																																																																																															
10 B	3.607209	2.872968	1.731531	2.948894	0.000000																																																																																																														

 <p>6. -1625.59210501 Cs +17.2</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>11 B</td> <td>1.744292</td> <td>2.907843</td> <td>2.945782</td> <td>1.733574</td> <td>3.437265</td> </tr> <tr> <td></td> <td>1</td> <td>2</td> <td>3</td> <td>4</td> <td>5</td> </tr> <tr> <td>1 B</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>2 B</td> <td>1.844833</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 B</td> <td>3.579475</td> <td>2.911812</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 C</td> <td>2.801164</td> <td>3.053262</td> <td>1.630403</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 B</td> <td>1.844840</td> <td>2.679700</td> <td>2.911819</td> <td>1.665495</td> <td>0.000000</td> </tr> <tr> <td>6 B</td> <td>1.757431</td> <td>1.806997</td> <td>2.879708</td> <td>2.714585</td> <td>2.829039</td> </tr> <tr> <td>7 B</td> <td>1.757474</td> <td>2.829025</td> <td>2.879624</td> <td>1.745742</td> <td>1.806963</td> </tr> <tr> <td>8 B</td> <td>1.750122</td> <td>1.742763</td> <td>3.433530</td> <td>2.936203</td> <td>1.742866</td> </tr> <tr> <td>9 B</td> <td>2.896423</td> <td>2.860319</td> <td>1.751706</td> <td>1.732920</td> <td>2.860247</td> </tr> <tr> <td>10 Mn</td> <td>3.013505</td> <td>2.200769</td> <td>1.948431</td> <td>2.189191</td> <td>2.200975</td> </tr> <tr> <td>11 C</td> <td>2.801230</td> <td>1.665609</td> <td>1.630410</td> <td>2.443800</td> <td>3.053362</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>1.768200</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 B</td> <td>2.920350</td> <td>2.920378</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>9 B</td> <td>1.745099</td> <td>1.744957</td> <td>3.634356</td> <td>0.000000</td> <td></td> </tr> <tr> <td>10 Mn</td> <td>3.218060</td> <td>3.218088</td> <td>1.957185</td> <td>3.045078</td> <td>0.000000</td> </tr> <tr> <td>11 C</td> <td>1.745801</td> <td>2.714539</td> <td>2.936291</td> <td>1.732948</td> <td>2.189152</td> </tr> </tbody> </table>		1	2	3	4	5	11 B	1.744292	2.907843	2.945782	1.733574	3.437265		1	2	3	4	5	1 B	0.000000					2 B	1.844833	0.000000				3 B	3.579475	2.911812	0.000000			4 C	2.801164	3.053262	1.630403	0.000000		5 B	1.844840	2.679700	2.911819	1.665495	0.000000	6 B	1.757431	1.806997	2.879708	2.714585	2.829039	7 B	1.757474	2.829025	2.879624	1.745742	1.806963	8 B	1.750122	1.742763	3.433530	2.936203	1.742866	9 B	2.896423	2.860319	1.751706	1.732920	2.860247	10 Mn	3.013505	2.200769	1.948431	2.189191	2.200975	11 C	2.801230	1.665609	1.630410	2.443800	3.053362		6	7	8	9	10	6 B	0.000000					7 B	1.768200	0.000000				8 B	2.920350	2.920378	0.000000			9 B	1.745099	1.744957	3.634356	0.000000		10 Mn	3.218060	3.218088	1.957185	3.045078	0.000000	11 C	1.745801	2.714539	2.936291	1.732948	2.189152
	1	2	3	4	5																																																																																																																										
11 B	1.744292	2.907843	2.945782	1.733574	3.437265																																																																																																																										
	1	2	3	4	5																																																																																																																										
1 B	0.000000																																																																																																																														
2 B	1.844833	0.000000																																																																																																																													
3 B	3.579475	2.911812	0.000000																																																																																																																												
4 C	2.801164	3.053262	1.630403	0.000000																																																																																																																											
5 B	1.844840	2.679700	2.911819	1.665495	0.000000																																																																																																																										
6 B	1.757431	1.806997	2.879708	2.714585	2.829039																																																																																																																										
7 B	1.757474	2.829025	2.879624	1.745742	1.806963																																																																																																																										
8 B	1.750122	1.742763	3.433530	2.936203	1.742866																																																																																																																										
9 B	2.896423	2.860319	1.751706	1.732920	2.860247																																																																																																																										
10 Mn	3.013505	2.200769	1.948431	2.189191	2.200975																																																																																																																										
11 C	2.801230	1.665609	1.630410	2.443800	3.053362																																																																																																																										
	6	7	8	9	10																																																																																																																										
6 B	0.000000																																																																																																																														
7 B	1.768200	0.000000																																																																																																																													
8 B	2.920350	2.920378	0.000000																																																																																																																												
9 B	1.745099	1.744957	3.634356	0.000000																																																																																																																											
10 Mn	3.218060	3.218088	1.957185	3.045078	0.000000																																																																																																																										
11 C	1.745801	2.714539	2.936291	1.732948	2.189152																																																																																																																										
 <p>7. -1625.58973940 +18.7</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>3.456726</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 B</td> <td>2.974716</td> <td>1.724485</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 B</td> <td>1.752777</td> <td>3.638613</td> <td>2.886007</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 C</td> <td>1.641137</td> <td>2.919949</td> <td>3.065795</td> <td>1.753770</td> <td>0.000000</td> </tr> <tr> <td>6 B</td> <td>2.916168</td> <td>1.728693</td> <td>2.685571</td> <td>2.894477</td> <td>1.649311</td> </tr> <tr> <td>7 C</td> <td>3.457154</td> <td>1.681656</td> <td>1.760432</td> <td>2.792823</td> <td>2.649444</td> </tr> <tr> <td>8 B</td> <td>2.861558</td> <td>2.896274</td> <td>2.816941</td> <td>1.746434</td> <td>1.710750</td> </tr> <tr> <td>9 B</td> <td>2.890485</td> <td>2.894989</td> <td>1.784982</td> <td>1.755464</td> <td>2.711653</td> </tr> <tr> <td>10 B</td> <td>1.719513</td> <td>3.030072</td> <td>1.750344</td> <td>1.825426</td> <td>2.581014</td> </tr> <tr> <td>11 Mn</td> <td>1.973615</td> <td>1.953757</td> <td>2.221122</td> <td>3.049896</td> <td>2.182520</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 C</td> <td>1.768372</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 B</td> <td>1.827169</td> <td>1.668773</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>9 B</td> <td>2.853468</td> <td>1.695600</td> <td>1.778898</td> <td>0.000000</td> <td></td> </tr> <tr> <td>10 B</td> <td>3.198017</td> <td>2.805821</td> <td>2.833443</td> <td>1.810854</td> <td>0.000000</td> </tr> <tr> <td>11 Mn</td> <td>2.164905</td> <td>2.877959</td> <td>3.186214</td> <td>3.196918</td> <td>2.265626</td> </tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.456726	0.000000				3 B	2.974716	1.724485	0.000000			4 B	1.752777	3.638613	2.886007	0.000000		5 C	1.641137	2.919949	3.065795	1.753770	0.000000	6 B	2.916168	1.728693	2.685571	2.894477	1.649311	7 C	3.457154	1.681656	1.760432	2.792823	2.649444	8 B	2.861558	2.896274	2.816941	1.746434	1.710750	9 B	2.890485	2.894989	1.784982	1.755464	2.711653	10 B	1.719513	3.030072	1.750344	1.825426	2.581014	11 Mn	1.973615	1.953757	2.221122	3.049896	2.182520		6	7	8	9	10	6 B	0.000000					7 C	1.768372	0.000000				8 B	1.827169	1.668773	0.000000			9 B	2.853468	1.695600	1.778898	0.000000		10 B	3.198017	2.805821	2.833443	1.810854	0.000000	11 Mn	2.164905	2.877959	3.186214	3.196918	2.265626												
	1	2	3	4	5																																																																																																																										
1 B	0.000000																																																																																																																														
2 B	3.456726	0.000000																																																																																																																													
3 B	2.974716	1.724485	0.000000																																																																																																																												
4 B	1.752777	3.638613	2.886007	0.000000																																																																																																																											
5 C	1.641137	2.919949	3.065795	1.753770	0.000000																																																																																																																										
6 B	2.916168	1.728693	2.685571	2.894477	1.649311																																																																																																																										
7 C	3.457154	1.681656	1.760432	2.792823	2.649444																																																																																																																										
8 B	2.861558	2.896274	2.816941	1.746434	1.710750																																																																																																																										
9 B	2.890485	2.894989	1.784982	1.755464	2.711653																																																																																																																										
10 B	1.719513	3.030072	1.750344	1.825426	2.581014																																																																																																																										
11 Mn	1.973615	1.953757	2.221122	3.049896	2.182520																																																																																																																										
	6	7	8	9	10																																																																																																																										
6 B	0.000000																																																																																																																														
7 C	1.768372	0.000000																																																																																																																													
8 B	1.827169	1.668773	0.000000																																																																																																																												
9 B	2.853468	1.695600	1.778898	0.000000																																																																																																																											
10 B	3.198017	2.805821	2.833443	1.810854	0.000000																																																																																																																										
11 Mn	2.164905	2.877959	3.186214	3.196918	2.265626																																																																																																																										
	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr> <td>1 B</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>2 B</td> <td>1.751008</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 B</td> <td>3.617897</td> <td>3.478286</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 B</td> <td>2.910432</td> <td>3.636989</td> <td>1.734768</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 C</td> <td>1.695739</td> <td>2.791773</td> <td>2.779015</td> <td>1.673948</td> <td>0.000000</td> </tr> <tr> <td>6 B</td> <td>1.846116</td> <td>1.745061</td> <td>2.950039</td> <td>2.893386</td> <td>2.705286</td> </tr> <tr> <td>7 B</td> <td>1.748024</td> <td>2.901108</td> <td>2.874048</td> <td>1.770113</td> <td>1.697289</td> </tr> <tr> <td>8 B</td> <td>1.821366</td> <td>1.716297</td> <td>2.996644</td> <td>2.872175</td> <td>1.713488</td> </tr> <tr> <td>9 C</td> <td>2.786096</td> <td>2.936482</td> <td>1.645425</td> <td>1.740181</td> <td>2.563720</td> </tr> <tr> <td>10 B</td> <td>2.933183</td> <td>3.028479</td> <td>1.711469</td> <td>1.805900</td> <td>1.753122</td> </tr> <tr> <td>11 Mn</td> <td>3.011987</td> <td>1.965756</td> <td>1.970141</td> <td>3.017346</td> <td>3.049430</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>1.794475</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 B</td> <td>2.679482</td> <td>2.811705</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>9 C</td> <td>1.670910</td> <td>1.701139</td> <td>3.065194</td> <td>0.000000</td> <td></td> </tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.751008	0.000000				3 B	3.617897	3.478286	0.000000			4 B	2.910432	3.636989	1.734768	0.000000		5 C	1.695739	2.791773	2.779015	1.673948	0.000000	6 B	1.846116	1.745061	2.950039	2.893386	2.705286	7 B	1.748024	2.901108	2.874048	1.770113	1.697289	8 B	1.821366	1.716297	2.996644	2.872175	1.713488	9 C	2.786096	2.936482	1.645425	1.740181	2.563720	10 B	2.933183	3.028479	1.711469	1.805900	1.753122	11 Mn	3.011987	1.965756	1.970141	3.017346	3.049430		6	7	8	9	10	6 B	0.000000					7 B	1.794475	0.000000				8 B	2.679482	2.811705	0.000000			9 C	1.670910	1.701139	3.065194	0.000000																									
	1	2	3	4	5																																																																																																																										
1 B	0.000000																																																																																																																														
2 B	1.751008	0.000000																																																																																																																													
3 B	3.617897	3.478286	0.000000																																																																																																																												
4 B	2.910432	3.636989	1.734768	0.000000																																																																																																																											
5 C	1.695739	2.791773	2.779015	1.673948	0.000000																																																																																																																										
6 B	1.846116	1.745061	2.950039	2.893386	2.705286																																																																																																																										
7 B	1.748024	2.901108	2.874048	1.770113	1.697289																																																																																																																										
8 B	1.821366	1.716297	2.996644	2.872175	1.713488																																																																																																																										
9 C	2.786096	2.936482	1.645425	1.740181	2.563720																																																																																																																										
10 B	2.933183	3.028479	1.711469	1.805900	1.753122																																																																																																																										
11 Mn	3.011987	1.965756	1.970141	3.017346	3.049430																																																																																																																										
	6	7	8	9	10																																																																																																																										
6 B	0.000000																																																																																																																														
7 B	1.794475	0.000000																																																																																																																													
8 B	2.679482	2.811705	0.000000																																																																																																																												
9 C	1.670910	1.701139	3.065194	0.000000																																																																																																																											

<p>8. -1625.58508256 +21.6</p>	<p>10 B 3.202033 2.846413 1.765295 2.567800 0.000000 11 Mn 2.195830 3.175868 2.227626 2.178634 2.235784</p>
	<p>1 2 3 4 5</p> <p>1 B 0.000000 2 C 1.773232 0.000000 3 B 3.682466 2.934008 0.000000 4 B 2.913890 3.071824 1.729445 0.000000 5 B 1.841188 2.569381 3.031131 1.763877 0.000000 6 B 1.775358 1.731463 2.924830 2.820210 2.846009 7 B 1.766585 2.715656 2.923896 1.790834 1.825572 8 C 1.648267 1.535432 3.334653 2.850109 1.603944 9 B 2.935094 2.789040 1.765774 1.825911 2.929850 10 Mn 3.076794 2.177071 1.967944 2.253791 2.257231 11 B 2.916242 1.662071 1.747986 2.683327 3.194929</p> <p>6 7 8 9 10</p> <p>6 B 0.000000 7 B 1.780291 0.000000 8 C 2.726782 2.736932 0.000000 9 B 1.748299 1.769909 3.440848 0.000000 10 Mn 3.209411 3.218982 1.906554 3.029013 0.000000 11 B 1.813853 2.845274 2.802867 1.845113 2.198282</p>
<p>9. -1625.58481346 +21.7</p>  <p>10. -1625.58316800 Cs(C_{2v}-like) +22.8</p>	<p>1 2 3 4 5</p> <p>1 B 0.000000 2 B 3.000473 0.000000 3 B 3.470027 1.721354 0.000000 4 B 1.721301 3.213086 3.000823 0.000000 5 C 1.698939 2.776890 3.480064 1.754555 0.000000 6 B 2.883999 1.781189 2.879975 2.839565 1.676619 7 C 3.485574 1.756959 1.695584 2.781310 2.665495 8 B 2.883425 2.838221 2.879271 1.782476 1.676348 9 B 2.999838 2.700500 1.720322 1.740851 2.776942 10 Mn 1.965258 2.229161 1.966018 2.235662 2.896342 11 B 1.722321 1.741047 3.001592 2.700900 1.754718</p> <p>6 7 8 9 10</p> <p>6 B 0.000000 7 C 1.677402 0.000000 8 B 1.808700 1.677118 0.000000 9 B 2.838891 1.757321 1.781396 0.000000 10 Mn 3.170145 2.898523 3.172126 2.233726 0.000000 11 B 1.782527 2.781424 2.839319 3.213323 2.231062</p>

 <p>11. -1625.58010255 Cs +22.7</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>2.905972</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.021526</td><td>1.812187</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.905941</td><td>1.795900</td><td>2.858909</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>3.343779</td><td>2.733211</td><td>1.622149</td><td>2.733309</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.731812</td><td>2.838444</td><td>3.224512</td><td>1.792196</td><td>2.859399</td></tr> <tr><td>7 B</td><td>1.731918</td><td>1.792266</td><td>1.747380</td><td>2.838552</td><td>2.859391</td></tr> <tr><td>8 B</td><td>3.021412</td><td>2.858881</td><td>2.722400</td><td>1.812243</td><td>1.622287</td></tr> <tr><td>9 Mn</td><td>1.987091</td><td>3.196105</td><td>2.237738</td><td>3.196134</td><td>1.893223</td></tr> <tr><td>10 B</td><td>1.766528</td><td>1.756223</td><td>2.922792</td><td>1.756172</td><td>3.458942</td></tr> <tr><td>11 C</td><td>3.514495</td><td>1.690343</td><td>1.775285</td><td>1.690502</td><td>1.569833</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.697800</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.747277</td><td>3.224564</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Mn</td><td>2.247474</td><td>2.247516</td><td>2.237667</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.837089</td><td>1.837201</td><td>2.922734</td><td>3.044709</td><td>0.000000</td></tr> <tr><td>11 C</td><td>2.790955</td><td>2.790936</td><td>1.775498</td><td>2.913556</td><td>2.806251</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.905972	0.000000				3 B	3.021526	1.812187	0.000000			4 B	2.905941	1.795900	2.858909	0.000000		5 C	3.343779	2.733211	1.622149	2.733309	0.000000	6 B	1.731812	2.838444	3.224512	1.792196	2.859399	7 B	1.731918	1.792266	1.747380	2.838552	2.859391	8 B	3.021412	2.858881	2.722400	1.812243	1.622287	9 Mn	1.987091	3.196105	2.237738	3.196134	1.893223	10 B	1.766528	1.756223	2.922792	1.756172	3.458942	11 C	3.514495	1.690343	1.775285	1.690502	1.569833		6	7	8	9	10	6 B	0.000000					7 B	2.697800	0.000000				8 B	1.747277	3.224564	0.000000			9 Mn	2.247474	2.247516	2.237667	0.000000		10 B	1.837089	1.837201	2.922734	3.044709	0.000000	11 C	2.790955	2.790936	1.775498	2.913556	2.806251
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	2.905972	0.000000																																																																																																																	
3 B	3.021526	1.812187	0.000000																																																																																																																
4 B	2.905941	1.795900	2.858909	0.000000																																																																																																															
5 C	3.343779	2.733211	1.622149	2.733309	0.000000																																																																																																														
6 B	1.731812	2.838444	3.224512	1.792196	2.859399																																																																																																														
7 B	1.731918	1.792266	1.747380	2.838552	2.859391																																																																																																														
8 B	3.021412	2.858881	2.722400	1.812243	1.622287																																																																																																														
9 Mn	1.987091	3.196105	2.237738	3.196134	1.893223																																																																																																														
10 B	1.766528	1.756223	2.922792	1.756172	3.458942																																																																																																														
11 C	3.514495	1.690343	1.775285	1.690502	1.569833																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	2.697800	0.000000																																																																																																																	
8 B	1.747277	3.224564	0.000000																																																																																																																
9 Mn	2.247474	2.247516	2.237667	0.000000																																																																																																															
10 B	1.837089	1.837201	2.922734	3.044709	0.000000																																																																																																														
11 C	2.790955	2.790936	1.775498	2.913556	2.806251																																																																																																														
 <p>12. -1625.57576002 +27.4</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 C</td><td>2.763992</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.854705</td><td>2.759366</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.792238</td><td>1.575278</td><td>2.819476</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.640326</td><td>2.845338</td><td>1.886940</td><td>1.872275</td><td>0.000000</td></tr> <tr><td>6 Mn</td><td>2.218495</td><td>3.195985</td><td>3.107123</td><td>2.104445</td><td>2.218705</td></tr> <tr><td>7 B</td><td>1.818074</td><td>1.608716</td><td>1.785361</td><td>2.572822</td><td>2.905284</td></tr> <tr><td>8 B</td><td>3.669489</td><td>3.244009</td><td>3.815751</td><td>1.675908</td><td>2.179138</td></tr> <tr><td>9 C</td><td>1.614385</td><td>3.397697</td><td>1.616984</td><td>2.773170</td><td>1.608006</td></tr> <tr><td>10 B</td><td>1.800417</td><td>1.629218</td><td>2.868643</td><td>1.858253</td><td>2.960049</td></tr> <tr><td>11 B</td><td>2.830098</td><td>1.612682</td><td>1.779406</td><td>1.849831</td><td>1.876302</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 Mn</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.347591</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.873446</td><td>4.071174</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.954416</td><td>2.778837</td><td>3.092581</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.180289</td><td>1.857905</td><td>3.051991</td><td>2.828862</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.332116</td><td>1.822971</td><td>3.222736</td><td>2.769901</td><td>2.651262</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	2.763992	0.000000				3 B	1.854705	2.759366	0.000000			4 B	2.792238	1.575278	2.819476	0.000000		5 B	2.640326	2.845338	1.886940	1.872275	0.000000	6 Mn	2.218495	3.195985	3.107123	2.104445	2.218705	7 B	1.818074	1.608716	1.785361	2.572822	2.905284	8 B	3.669489	3.244009	3.815751	1.675908	2.179138	9 C	1.614385	3.397697	1.616984	2.773170	1.608006	10 B	1.800417	1.629218	2.868643	1.858253	2.960049	11 B	2.830098	1.612682	1.779406	1.849831	1.876302		6	7	8	9	10	6 Mn	0.000000					7 B	3.347591	0.000000				8 B	1.873446	4.071174	0.000000			9 C	1.954416	2.778837	3.092581	0.000000		10 B	2.180289	1.857905	3.051991	2.828862	0.000000	11 B	3.332116	1.822971	3.222736	2.769901	2.651262
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 C	2.763992	0.000000																																																																																																																	
3 B	1.854705	2.759366	0.000000																																																																																																																
4 B	2.792238	1.575278	2.819476	0.000000																																																																																																															
5 B	2.640326	2.845338	1.886940	1.872275	0.000000																																																																																																														
6 Mn	2.218495	3.195985	3.107123	2.104445	2.218705																																																																																																														
7 B	1.818074	1.608716	1.785361	2.572822	2.905284																																																																																																														
8 B	3.669489	3.244009	3.815751	1.675908	2.179138																																																																																																														
9 C	1.614385	3.397697	1.616984	2.773170	1.608006																																																																																																														
10 B	1.800417	1.629218	2.868643	1.858253	2.960049																																																																																																														
11 B	2.830098	1.612682	1.779406	1.849831	1.876302																																																																																																														
	6	7	8	9	10																																																																																																														
6 Mn	0.000000																																																																																																																		
7 B	3.347591	0.000000																																																																																																																	
8 B	1.873446	4.071174	0.000000																																																																																																																
9 C	1.954416	2.778837	3.092581	0.000000																																																																																																															
10 B	2.180289	1.857905	3.051991	2.828862	0.000000																																																																																																														
11 B	3.332116	1.822971	3.222736	2.769901	2.651262																																																																																																														
 <p>13. -1625.56821479 Cs +32.2</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>2.102380</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.285581</td><td>2.067759</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.850894</td><td>2.882359</td><td>1.775441</td><td>0.000000</td><td></td></tr> <tr><td>5 Mn</td><td>2.085015</td><td>3.190338</td><td>3.406096</td><td>2.170810</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.861323</td><td>2.067591</td><td>2.703900</td><td>2.845980</td><td>3.405955</td></tr> <tr><td>7 B</td><td>1.779526</td><td>2.882221</td><td>2.846026</td><td>1.829900</td><td>2.170800</td></tr> <tr><td>8 C</td><td>1.609100</td><td>1.625317</td><td>2.838668</td><td>2.745147</td><td>1.949392</td></tr> <tr><td>9 B</td><td>2.959100</td><td>2.758961</td><td>1.808626</td><td>1.770018</td><td>3.424735</td></tr> <tr><td>10 B</td><td>2.711000</td><td>2.102658</td><td>1.861456</td><td>1.779517</td><td>2.085017</td></tr> <tr><td>11 C</td><td>2.848967</td><td>1.628100</td><td>1.581057</td><td>2.688790</td><td>3.895803</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.775258</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.838672</td><td>2.745165</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.808584</td><td>1.769977</td><td>3.423902</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.102380	0.000000				3 B	3.285581	2.067759	0.000000			4 B	2.850894	2.882359	1.775441	0.000000		5 Mn	2.085015	3.190338	3.406096	2.170810	0.000000	6 B	1.861323	2.067591	2.703900	2.845980	3.405955	7 B	1.779526	2.882221	2.846026	1.829900	2.170800	8 C	1.609100	1.625317	2.838668	2.745147	1.949392	9 B	2.959100	2.758961	1.808626	1.770018	3.424735	10 B	2.711000	2.102658	1.861456	1.779517	2.085017	11 C	2.848967	1.628100	1.581057	2.688790	3.895803		6	7	8	9	10	6 B	0.000000					7 B	1.775258	0.000000				8 C	2.838672	2.745165	0.000000			9 B	1.808584	1.769977	3.423902	0.000000													
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	2.102380	0.000000																																																																																																																	
3 B	3.285581	2.067759	0.000000																																																																																																																
4 B	2.850894	2.882359	1.775441	0.000000																																																																																																															
5 Mn	2.085015	3.190338	3.406096	2.170810	0.000000																																																																																																														
6 B	1.861323	2.067591	2.703900	2.845980	3.405955																																																																																																														
7 B	1.779526	2.882221	2.846026	1.829900	2.170800																																																																																																														
8 C	1.609100	1.625317	2.838668	2.745147	1.949392																																																																																																														
9 B	2.959100	2.758961	1.808626	1.770018	3.424735																																																																																																														
10 B	2.711000	2.102658	1.861456	1.779517	2.085017																																																																																																														
11 C	2.848967	1.628100	1.581057	2.688790	3.895803																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.775258	0.000000																																																																																																																	
8 C	2.838672	2.745165	0.000000																																																																																																																
9 B	1.808584	1.769977	3.423902	0.000000																																																																																																															

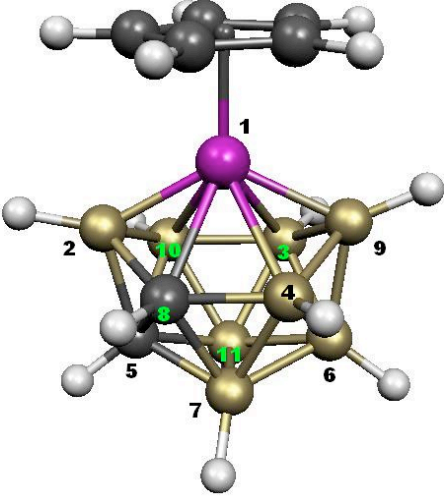
	10 B	3.285582	2.850880	1.609048	2.959128	0.000000
	11 C	1.581011	2.688692	2.979441	1.657020	2.849100
		1	2	3	4	5
 <p>14. -1625.56566578 +33.8</p>	1 Mn	0.000000				
	2 B	1.950380	0.000000			
	3 B	2.256802	3.001673	0.000000		
	4 B	2.202567	2.951338	2.692276	0.000000	
	5 C	2.887700	1.688044	2.761905	2.756254	0.000000
	6 B	3.035437	3.624830	1.835056	1.849660	2.792148
	7 B	3.203202	2.906613	2.824663	1.809451	1.698075
	8 C	2.142135	1.646726	3.064269	1.652385	1.656365
	9 B	1.973235	3.465465	1.725746	1.742538	3.487812
	10 B	2.235292	1.722766	1.747832	3.195787	1.749306
	11 B	3.198827	2.899226	1.783135	2.842798	1.681348
		6	7	8	9	10
6 B	0.000000					
7 B	1.736811	0.000000				
8 C	2.784913	1.746764	0.000000			
9 B	1.765417	2.908887	2.906137	0.000000		
10 B	2.925502	2.858141	2.569084	3.007840	0.000000	
11 B	1.766636	1.784960	2.710683	2.905382	1.815408	

Table 3. Energy ranking

	Initial structure	Final energy (a.u.)	D kcal/mole	Remarks
1	2-TricapCubeB_Mn_v4_C2_u	-1625.61945329	0.00	
2	1-PentaCapTrPr_Mn_v4_C2_v66b	-1625.61945328	0.00	
3	2-TricapCubeB_Mn_v4_C2_a	-1625.61945328	0.00	
4	3-OhfusettoPentBipyr_Mn_v4_C2_g_r-24	-1625.61945323	0.00	
5	4-Icos-1vx_Mn_v5a_C2_h_r-25	-1625.61945320	0.00	
6	3-OhfusettoPentBipyr_Mn_v6a_C2_c	-1625.61945318	0.00	
7	2-TricapCubeA_Mn_v4a_C2_v55b	-1625.61945309	0.00	
8	4-Icos-1vx_Mn_v6_C2_f_r-25	-1625.61945309	0.00	
9	1-PentaCapTrPr_Mn_v6_C2_q	-1625.61945293	0.00	
10	1-PentaCapTrPr_Mn_v4_C2_v33	-1625.61945031	0.00	
11	4-Icos-1vx_Mn_v6_C2_f_i-25	-1625.61941252	0.03	
12	4-Icos-1vx_Mn_v5a_C2_h_i-25	-1625.61937987	0.05	
13	3-OhfusettoPentBipyr_Mn_v4_C2_g_i-24	-1625.61937824	0.05	
14	1-PentaCapTrPr_Mn_v3_C2_v44	-1625.60777112	7.33	
15	4-Icos-1vx_Mn_v5b_C2_f	-1625.60777110	7.33	
16	4-Icos-1vx_Mn_v5b_C2_w	-1625.60777054	7.33	
17	1-PentaCapTrPr_Mn_v4_C2_v66a	-1625.60776897	7.33	
18	1-PentaCapTrPr_Mn_v6_C2_c	-1625.60776896	7.33	
19	2-TricapCubeA_Mn_v4b_C2_k	-1625.60776888	7.33	
20	1-PentaCapTrPr_Mn_v3_C2_v66c	-1625.60776881	7.33	
21	3-OhfusettoPentBipyr_Mn_v5_C2_v	-1625.60776881	7.33	
22	1-PentaCapTrPr_Mn_v4_C2_v63b	-1625.60776878	7.33	
23	4-Icos-1vx_Mn_v4_C2_zz	-1625.60776874	7.33	
24	4-Icos-1vx_Mn_v5a_C2_p	-1625.60776871	7.33	
25	2-TricapCubeB_Mn_v6_C2_w	-1625.60776870	7.33	
26	4-Icos-1vx_Mn_v5a_C2_d	-1625.60776868	7.33	
27	2-TricapCubeA_Mn_v4a_C2_v55a	-1625.60776859	7.33	
28	4-Icos-1vx_Mn_v6_C2_d	-1625.60776854	7.33	
29	4-Icos-1vx_Mn_v5b_C2_u_r-494-77	-1625.60776848	7.33	
30	2-TricapCubeA_Mn_v4a_C2_v54f	-1625.60776843	7.33	
31	4-Icos-1vx_Mn_v5a_C2_zs	-1625.60775844	7.34	
32	3-OhfusettoPentBipyr_Mn_v6a_C2_zz	-1625.60775770	7.34	
33	4-Icos-1vx_Mn_v5b_C2_a_r-274	-1625.60732896	7.61	
34	4-Icos-1vx_Mn_v5b_C2_l	-1625.60732896	7.61	
35	4-Icos-1vx_Mn_v4_C2_y	-1625.60732895	7.61	
36	4-Icos-1vx_Mn_v5a_C2_f	-1625.60732895	7.61	
37	2-TricapCubeB_Mn_v4_C2_c	-1625.60732894	7.61	
38	2-TricapCubeB_Mn_v4_C2_g	-1625.60732894	7.61	

39	2-TricapCubeA_Mn_v4a_C2_v54c	-1625.60732893	7.61	
40	4-Icos-1vx_Mn_v5b_C2_a_r-28	-1625.60732893	7.61	
41	1-PentaCapTrPr_Mn_v6_C2_a	-1625.60732892	7.61	
42	4-Icos-1vx_Mn_v6_C2_e	-1625.60732860	7.61	
43	3-OhfusettoPentBipyr_Mn_v6b_C2_v	-1625.60732782	7.61	
44	3-OhfusettoPentBipyr_Mn_v4_C2_p	-1625.60689863	7.88	
45	2-TricapCubeB_Mn_v4_C2_l	-1625.60169400	11.14	
46	2-TricapCubeA_Mn_v4a_C2_v54d	-1625.60169399	11.14	
47	4-Icos-1vx_Mn_v5a_C2_zl	-1625.60169399	11.14	
48	2-TricapCubeB_Mn_v4_C2_f	-1625.60169396	11.14	
49	2-TricapCubeB_Mn_v6_C2_r	-1625.60169394	11.14	
50	1-PentaCapTrPr_Mn_v6_C2_l	-1625.60169393	11.14	
51	1-PentaCapTrPr_Mn_v4_C2_v66d	-1625.60169389	11.14	
52	4-Icos-1vx_Mn_v4_C2_b	-1625.60169389	11.14	
53	2-TricapCubeB_Mn_v6_C2_l	-1625.60169386	11.14	
54	1-PentaCapTrPr_Mn_v6_C2_j	-1625.60169385	11.14	
55	3-OhfusettoPentBipyr_Mn_v6b_C2_r	-1625.60169375	11.14	
56	2-TricapCubeA_Mn_v4a_C2_v54b	-1625.60169366	11.14	
57	2-TricapCubeB_Mn_v6_C2_q	-1625.60169289	11.14	
58	4-Icos-1vx_Mn_v6_C2_c	-1625.60169261	11.14	
59	4-Icos-1vx_Mn_v4_C2_h_r-120	-1625.59638607	14.47	
60	4-Icos-1vx_Mn_v5a_C2_zi_r-20	-1625.59638552	14.48	
61	4-Icos-1vx_Mn_v5c_C2_v	-1625.59638204	14.48	
62	2-TricapCubeA_Mn_v4a_C2_v44	-1625.59637422	14.48	
63	2-TricapCubeB_Mn_v6_C2_b	-1625.59634819	14.50	
64	4-Icos-1vx_Mn_v6_C2_o_i-10	-1625.59634296	14.50	
65	2-TricapCubeA_Mn_v4b_C2_t	-1625.59634143	14.50	
66	4-Icos-1vx_Mn_v5a_C2_o	-1625.59634008	14.50	
67	4-Icos-1vx_Mn_v6_C2_o_r-10	-1625.59634003	14.50	
68	2-TricapCubeB_Mn_v4_C2_v	-1625.59633957	14.50	
69	4-Icos-1vx_Mn_v5a_C2_zi_i-20	-1625.59628121	14.54	
70	4-Icos-1vx_Mn_v5a_C2_q	-1625.59210501	17.16	
71	3-OhfusettoPentBipyr_Mn_v6b_C2_za	-1625.59210486	17.16	
72	1-PentaCapTrPr_Mn_v6_C2_o	-1625.59210480	17.16	
73	4-Icos-1vx_Mn_v6_C2_n	-1625.59210433	17.16	
74	2-TricapCubeA_Mn_v4b_C2_s	-1625.58973940	18.65	
75	2-TricapCubeA_Mn_v4a_C2_v54k	-1625.58973731	18.65	
76	1-PentaCapTrPr_Mn_v6_C2_i	-1625.58973716	18.65	
77	1-PentaCapTrPr_Mn_v6_C2_p	-1625.58973709	18.65	
78	4-Icos-1vx_Mn_v5a_C2_n	-1625.58973709	18.65	
79	4-Icos-1vx_Mn_v5a_C2_zp	-1625.58972733	18.65	

80	2-TricapCubeB_Mn_v6_C2_o_cont	-1625.58972504	18.65	
81	4-Icos-1vx_Mn_v5c_C2_zz_r-262	-1625.58508354	21.57	
82	4-Icos-1vx_Mn_v5a_C2_m	-1625.58508273	21.57	
83	4-Icos-1vx_Mn_v5a_C2_zd	-1625.58508265	21.57	
84	4-Icos-1vx_Mn_v4_C2_l	-1625.58508263	21.57	
85	4-Icos-1vx_Mn_v6_C2_l	-1625.58508256	21.57	
86	3-OhfusetopentBipyr_Mn_v6b_C2_q	-1625.58508255	21.57	
87	4-Icos-1vx_Mn_v5a_C2_zq	-1625.58481346	21.74	C-C
88	3-OhfusetopentBipyr_Mn_v6b_C2_g	-1625.58481203	21.74	C-C
89	1-PentaCapTrPr_Mn_v6_C2_e	-1625.58481199	21.74	C-C
90	1-PentaCapTrPr_Mn_v6_C2_n	-1625.58481198	21.74	C-C
91	4-Icos-1vx_Mn_v5a_C2_i	-1625.58481188	21.74	C-C
92	2-TricapCubeA_Mn_v4a_C2_v54e	-1625.58481183	21.74	C-C
93	4-Icos-1vx_Mn_v4_C2_p	-1625.58481177	21.74	C-C
94	4-Icos-1vx_Mn_v5a_C2_a	-1625.58481174	21.74	C-C
95	2-TricapCubeB_Mn_v6_C2_n	-1625.58481166	21.74	C-C
96	1-PentaCapTrPr_Mn_v4_C2_v63a	-1625.58481161	21.74	C-C
97	2-TricapCubeA_Mn_v4a_C2_v55c	-1625.58481155	21.74	C-C
98	4-Icos-1vx_Mn_v6_C2_b	-1625.58481101	21.74	C-C
99	2-TricapCubeB_Mn_v6_C2_d	-1625.58480961	21.74	C-C
100	1-PentaCapTrPr_Mn_v3_C2_v64	-1625.58480663	21.74	C-C
101	2-TricapCubeA_Mn_v4a_C2_v54h	-1625.58316800	22.77	
102	4-Icos-1vx_Mn_v6_C2_i_r-13	-1625.58316763	22.77	
103	1-PentaCapTrPr_Mn_v6_C2_f	-1625.58316758	22.77	
104	2-TricapCubeB_Mn_v4_C2_k	-1625.58316472	22.77	
105	1-PentaCapTrPr_Mn_v4_C2_v44	-1625.58315518	22.78	
106	4-Icos-1vx_Mn_v6_C2_i_i-13	-1625.58314728	22.78	
107	1-PentaCapTrPr_Mn_v4_C2_v64a	-1625.58010255	24.69	C-C
108	1-PentaCapTrPr_Mn_v6_C2_b	-1625.58010255	24.69	C-C
109	4-Icos-1vx_Mn_v5a_C2_b	-1625.58010253	24.69	C-C
110	2-TricapCubeA_Mn_v4b_C2_o	-1625.58010242	24.69	C-C
111	4-Icos-1vx_Mn_v6_C2_a	-1625.58010237	24.69	C-C
112	2-TricapCubeB_Mn_v4_C2_b	-1625.58010232	24.69	C-C
113	2-TricapCubeB_Mn_v6_C2_i	-1625.58010232	24.69	C-C
114	4-Icos-1vx_Mn_v5a_C2_zo	-1625.58010228	24.69	C-C
115	2-TricapCubeA_Mn_v4a_C2_v54a	-1625.58010211	24.69	C-C
116	2-TricapCubeB_Mn_v6_C2_t	-1625.58010171	24.69	C-C
117	3-OhfusetopentBipyr_Mn_v6a_C2_l	-1625.58010167	24.69	C-C
118	1-PentaCapTrPr_Mn_v6_C2_t	-1625.57576002	27.42	
119	2-TricapCubeA_Mn_v4b_C2_m	-1625.57547411	27.60	
120	4-Icos-1vx_Mn_v5c_C2_o	-1625.56821488	32.15	

121	1-PentaCapTrPr_Mn_v3_C2_v43	-1625.56821486	32.15	
122	4-Icos-1vx_Mn_v5b_C2_e	-1625.56821479	32.15	
123	1-PentaCapTrPr_Mn_v4_C2_v63d	-1625.56821478	32.15	
124	1-PentaCapTrPr_Mn_v4_C2_v66e	-1625.56821475	32.15	
125	4-Icos-1vx_Mn_v4_C2_o	-1625.56821473	32.15	
126	4-Icos-1vx_Mn_v5b_C2_d	-1625.56821472	32.15	
127	4-Icos-1vx_Mn_v5a_C2_zm	-1625.56821468	32.15	
128	4-Icos-1vx_Mn_v5a_C2_e	-1625.56821454	32.15	
129	2-TricapCubeA_Mn_v4b_C2_i	-1625.56821449	32.15	
130	2-TricapCubeA_Mn_v4b_C2_h	-1625.56821024	32.16	
131	2-TricapCubeB_Mn_v6_C2_x	-1625.56566578	33.75	C-C
132	2-TricapCubeA_Mn_v4a_C2_v54j	-1625.56566562	33.75	C-C
133	3-OhfusettoPentBipyr_Mn_v4_C2_l	-1625.56566552	33.75	C-C
134	1-PentaCapTrPr_Mn_v6_C2_g	-1625.56566549	33.75	C-C
135	1-PentaCapTrPr_Mn_v6_C2_r	-1625.56566518	33.75	C-C
136	2-TricapCubeB_Mn_v6_C2_a	-1625.56566502	33.75	C-C
137	4-Icos-1vx_Mn_v6_C2_g	-1625.56566499	33.75	C-C
138	4-Icos-1vx_Mn_v5a_C2_j	-1625.56566445	33.75	C-C
139	4-Icos-1vx_Mn_v5a_C2_zf	-1625.56564916	33.76	C-C
140	4-Icos-1vx_Mn_v5a_C2_l	-1625.56556765	33.81	C-C
141	4-Icos-1vx_Mn_v6_C2_m	-1625.56556763	33.81	C-C
142	4-Icos-1vx_Mn_v5a_C2_zr	-1625.56556693	33.81	C-C
143	4-Icos-1vx_Mn_v5c_C2_f	-1625.56454494	34.45	
144	4-Icos-1vx_Mn_v5b_C2_m	-1625.56453933	34.46	
145	2-TricapCubeA_Mn_v4b_C2_l	-1625.56453877	34.46	
146	4-Icos-1vx_Mn_v4_C2_e	-1625.56453705	34.46	
147	2-TricapCubeB_Mn_v4_C2_m	-1625.56453657	34.46	
148	4-Icos-1vx_Mn_v5c_C2_j	-1625.56453552	34.46	
149	4-Icos-1vx_Mn_v4_C2_i	-1625.56453339	34.46	
150	4-Icos-1vx_Mn_v5a_C2_x	-1625.56453306	34.46	
151	4-Icos-1vx_Mn_v5b_C2_r	-1625.56453133	34.46	
152	4-Icos-1vx_Mn_v5a_C2_g	-1625.56453054	34.46	
153	4-Icos-1vx_Mn_v5c_C2_r	-1625.56452533	34.47	
154	4-Icos-1vx_Mn_v4_C2_q	-1625.56449967	34.48	
155	4-Icos-1vx_Mn_v4_C2_r	-1625.56261985	35.66	C-C
156	1-PentaCapTrPr_Mn_v4_C2_v63c	-1625.56261980	35.66	C-C
157	4-Icos-1vx_Mn_v5c_C2_n	-1625.56261978	35.66	C-C
158	4-Icos-1vx_Mn_v5a_C2_k	-1625.56261961	35.66	C-C
159	4-Icos-1vx_Mn_v6_C2_k	-1625.56261939	35.66	C-C
160	2-TricapCubeB_Mn_v4_C2_y	-1625.55740674	38.93	
161	3-OhfusettoPentBipyr_Mn_v6a_C2_x	-1625.55676376	39.34	

162	2-TricapCubeB_Mn_v6_C2_c	-1625.55675986	39.34	
163	1-PentaCapTrPr_Mn_v3_C2_v63a	-1625.55675963	39.34	
164	2-TricapCubeB_Mn_v6_C2_h	-1625.55582939	39.92	C-C
165	2-TricapCubeB_Mn_v4_C2_o	-1625.55582571	39.93	C-C
166	2-TricapCubeA_Mn_v4a_C2_v54i	-1625.55582533	39.93	C-C
167	4-Icos-1vx_Mn_v6_C2_h	-1625.55582373	39.93	C-C
168	3-OhfusetopentBipyr_Mn_v6a_C2_t_r-38	-1625.55580131	39.94	
169	3-OhfusetopentBipyr_Mn_v6b_C2_t	-1625.55580112	39.94	
170	3-OhfusetopentBipyr_Mn_v6b_C2_b	-1625.55580084	39.94	
171	1-PentaCapTrPr_Mn_v4_C2_v43	-1625.55580071	39.94	
172	2-TricapCubeB_Mn_v6_C2_j	-1625.55580061	39.94	
173	3-OhfusetopentBipyr_Mn_v5_C2_k	-1625.55491954	40.49	
174	3-OhfusetopentBipyr_Mn_v6b_C2_f	-1625.55491945	40.49	
175	3-OhfusetopentBipyr_Mn_v6a_C2_t_i-38	-1625.55454883	40.73	
176	2-TricapCubeB_Mn_v6_C2_m	-1625.55441867	40.81	
177	1-PentaCapTrPr_Mn_v6_C2_d	-1625.55441758	40.81	
178	1-PentaCapTrPr_Mn_v6_C2_m	-1625.55368376	41.27	
179	4-Icos-1vx_Mn_v6_C2_j_r-12	-1625.55342115	41.44	C-C
180	4-Icos-1vx_Mn_v6_C2_j_i-12	-1625.55340745	41.44	C-C
181	4-Icos-1vx_Mn_v5c_C2_h_r-306	-1625.55329961	41.51	
182	4-Icos-1vx_Mn_v5a_C2_u	-1625.55329958	41.51	
183	4-Icos-1vx_Mn_v5c_C2_h_r-119	-1625.55329524	41.51	
184	2-TricapCubeB_Mn_v4_C2_n	-1625.55329491	41.51	
185	2-TricapCubeB_Mn_v4_C2_zz	-1625.55329247	41.52	
186	4-Icos-1vx_Mn_v4_C2_t	-1625.55235655	42.10	
187	4-Icos-1vx_Mn_v4_C2_x	-1625.55235655	42.10	
188	4-Icos-1vx_Mn_v5b_C2_b	-1625.55235655	42.10	
189	4-Icos-1vx_Mn_v5b_C2_k	-1625.55235655	42.10	
190	4-Icos-1vx_Mn_v5c_C2_k	-1625.55235655	42.10	
191	4-Icos-1vx_Mn_v5a_C2_v	-1625.55235626	42.10	
192	2-TricapCubeA_Mn_v4b_C2_e	-1625.55235621	42.10	
193	4-Icos-1vx_Mn_v4_C2_k	-1625.55235598	42.10	
194	2-TricapCubeA_Mn_v4b_C2_x	-1625.55235508	42.10	
195	3-OhfusetopentBipyr_Mn_v5_C2_f	-1625.55172070	42.50	
196	2-TricapCubeB_Mn_v4_C2_e	-1625.55172065	42.50	
197	1-PentaCapTrPr_Mn_v4_C2_v64b	-1625.55172026	42.50	
198	3-OhfusetopentBipyr_Mn_v6a_C2_r	-1625.55171924	42.50	
199	1-PentaCapTrPr_Mn_v6_C2_u	-1625.55084232	43.05	
200	2-TricapCubeB_Mn_v4_C2_r	-1625.55083231	43.06	
201	2-TricapCubeA_Mn_v4b_C2_a	-1625.54936156	43.98	
202	4-Icos-1vx_Mn_v5a_C2_ze	-1625.54935590	43.99	

203	4-Icos-1vx_Mn_v5c_C2_m	-1625.54935526	43.99	
204	2-TricapCubeB_Mn_v6_C2_f	-1625.54891606	44.26	
205	3-OhfusetopentBipyr_Mn_v6a_C2_n	-1625.54891598	44.26	
206	2-TricapCubeB_Mn_v4_C2_i	-1625.54887930	44.29	
207	3-OhfusetopentBipyr_Mn_v5_C2_p	-1625.54884021	44.31	
208	2-TricapCubeB_Mn_v6_C2_y	-1625.54857321	44.48	
209	4-Icos-1vx_Mn_v5c_C2_u	-1625.54820568	44.71	
210	4-Icos-1vx_Mn_v5c_C2_w_r-204	-1625.54820508	44.71	
211	4-Icos-1vx_Mn_v5c_C2_d	-1625.54820275	44.71	
212	2-TricapCubeA_Mn_v4b_C2_c	-1625.54819481	44.71	
213	4-Icos-1vx_Mn_v5c_C2_a	-1625.54786405	44.92	
214	1-PentaCapTrPr_Mn_v3_C2_v66a	-1625.54606641	46.05	
215	2-TricapCubeB_Mn_v6_C2_e	-1625.54606615	46.05	
216	2-TricapCubeB_Mn_v6_C2_z	-1625.54606603	46.05	
217	4-Icos-1vx_Mn_v5a_C2_zh	-1625.54606583	46.05	
218	1-PentaCapTrPr_Mn_v4_C2_v66c	-1625.54606566	46.05	
219	2-TricapCubeB_Mn_v6_C2_zz	-1625.54544697	46.44	
220	3-OhfusetopentBipyr_Mn_v5_C2_l	-1625.54544189	46.44	
221	3-OhfusetopentBipyr_Mn_v4_C2_m	-1625.54544151	46.44	
222	3-OhfusetopentBipyr_Mn_v6a_C2_m	-1625.54544145	46.44	
223	1-PentaCapTrPr_Mn_v3_C2_v66d	-1625.54543815	46.44	
224	2-TricapCubeB_Mn_v6_C2_k	-1625.54543609	46.45	
225	2-TricapCubeA_Mn_v4b_C2_j	-1625.54532822	46.51	
226	4-Icos-1vx_Mn_v5b_C2_v	-1625.54532818	46.51	
227	4-Icos-1vx_Mn_v4_C2_d	-1625.54532785	46.51	
228	4-Icos-1vx_Mn_v5b_C2_o	-1625.54519323	46.60	
229	4-Icos-1vx_Mn_v4_C2_u	-1625.54519148	46.60	
230	4-Icos-1vx_Mn_v5a_C2_c	-1625.54519041	46.60	
231	3-OhfusetopentBipyr_Mn_v4_C2_u	-1625.54244626	48.32	
232	3-OhfusetopentBipyr_Mn_v5_C2_g	-1625.54045023	49.57	
233	3-OhfusetopentBipyr_Mn_v6a_C2_v	-1625.54045019	49.57	
234	4-Icos-1vx_Mn_v5c_C2_c_r-10	-1625.54044480	49.58	
235	2-TricapCubeB_Mn_v6_C2_u	-1625.53999448	49.86	
236	1-PentaCapTrPr_Mn_v3_C2_v66d	-1625.53999397	49.86	
237	3-OhfusetopentBipyr_Mn_v6a_C2_b	-1625.53999344	49.86	
238	2-TricapCubeB_Mn_v6_C2_g_r-10	-1625.53999236	49.86	
239	2-TricapCubeB_Mn_v6_C2_g	-1625.53998528	49.87	
240	2-TricapCubeB_Mn_v4_C2_j	-1625.53966020	50.07	C-C
241	3-OhfusetopentBipyr_Mn_v6a_C2_e	-1625.53916345	50.38	
242	1-PentaCapTrPr_Mn_v6_C2_s	-1625.53880811	50.60	
243	2-TricapCubeA_Mn_v4b_C2_q	-1625.53831405	50.91	

244	4-Icos-1vx_Mn_v5a_C2_zg	-1625.53831088	50.92	
245	2-TricapCubeB_Mn_v4_C2_q	-1625.53620305	52.24	C-C
246	3-OhfusetopentBipyr_Mn_v5_C2_d	-1625.53618557	52.25	C-C
247	4-Icos-1vx_Mn_v5a_C2_zb	-1625.53578735	52.50	
248	2-TricapCubeA_Mn_v4b_C2_w	-1625.53578721	52.50	
249	4-Icos-1vx_Mn_v5b_C2_q	-1625.53556359	52.64	
250	4-Icos-1vx_Mn_v4_C2_h i-120	-1625.53531349	52.80	
251	2-TricapCubeB_Mn_v4_C2_s	-1625.53510114	52.93	C-C
252	2-TricapCubeA_Mn_v4b_C2_p	-1625.53480688	53.12	C-C
253	4-Icos-1vx_Mn_v4_C2_a	-1625.53404484	53.59	C-C
254	4-Icos-1vx_Mn_v4_C2_z	-1625.53404458	53.59	
255	3-OhfusetopentBipyr_Mn_v6a_C2_h_r-13	-1625.53349593	53.94	
256	4-Icos-1vx_Mn_v5a_C2_s	-1625.53348783	53.94	
257	3-OhfusetopentBipyr_Mn_v6a_C2_y	-1625.53316579	54.15	
258	4-Icos-1vx_Mn_v5b_C2_h	-1625.53295880	54.28	
259	2-TricapCubeB_Mn_v4_C2_z	-1625.53292422	54.30	
260	2-TricapCubeB_Mn_v6_C2_v	-1625.52853119	57.05	
261	4-Icos-1vx_Mn_v4_C2_c	-1625.52853117	57.05	
262	2-TricapCubeB_Mn_v4_C2_x	-1625.52822358	57.25	C-C
263	3-OhfusetopentBipyr_Mn_v4_C2_t	-1625.52799575	57.39	
264	3-OhfusetopentBipyr_Mn_v5_C2_zz	-1625.52799567	57.39	
265	3-OhfusetopentBipyr_Mn_v6b_C2_l	-1625.52720226	57.89	
266	3-OhfusetopentBipyr_Mn_v6a_C2_u	-1625.52720189	57.89	
267	3-OhfusetopentBipyr_Mn_v4_C2_c	-1625.52638908	58.40	
268	3-OhfusetopentBipyr_Mn_v5_C2_m	-1625.52562471	58.88	
269	4-Icos-1vx_Mn_v5c_C2_e	-1625.52518771	59.15	C-C
270	2-TricapCubeA_Mn_v4b_C2_u	-1625.52518673	59.15	C-C
271	4-Icos-1vx_Mn_v5c_C2_s	-1625.52518605	59.15	C-C
272	2-TricapCubeA_Mn_v4b_C2_b	-1625.52518532	59.15	C-C
273	4-Icos-1vx_Mn_v5c_C2_i	-1625.52464318	59.49	
274	4-Icos-1vx_Mn_v5c_C2_y	-1625.52464047	59.50	
275	1-PentaCapTrPr_Mn_v3_C2_v64b	-1625.52393726	59.94	C-C
276	4-Icos-1vx_Mn_v5c_C2_c i-10	-1625.52141734	61.52	
277	3-OhfusetopentBipyr_Mn_v4_C2_d	-1625.52113050	61.70	
278	2-TricapCubeA_Mn_v4b_C2_n	-1625.51959151	62.66	
279	2-TricapCubeB_Mn_v4_C2_h	-1625.51958801	62.67	
280	4-Icos-1vx_Mn_v5b_C2_s	-1625.51894337	63.07	C-C
281	4-Icos-1vx_Mn_v4_C2_v	-1625.51894205	63.07	C-C
282	4-Icos-1vx_Mn_v5b_C2_i	-1625.51890554	63.09	C-C
283	4-Icos-1vx_Mn_v5a_C2_w	-1625.51837680	63.43	
284	1-PentaCapTrPr_Mn_v6_C2_k	-1625.51781329	63.78	C-C

285	4-Icos-1vx_Mn_v4_C2_f	-1625.51773951	63.83	
286	4-Icos-1vx_Mn_v5a_C2_zc	-1625.51773939	63.83	
287	1-PentaCapTrPr_Mn_v6_C2_h	-1625.51707921	64.24	C-C
288	2-TricapCubeB_Mn_v4_C2_w	-1625.51633599	64.71	
289	2-TricapCubeB_Mn_v4_C2_d	-1625.51394233	66.21	
290	2-TricapCubeB_Mn_v4_C2_p	-1625.51344624	66.52	C-C
291	4-Icos-1vx_Mn_v5a_C2_z	-1625.51344617	66.52	C-C
292	4-Icos-1vx_Mn_v5a_C2_zk	-1625.51344609	66.52	C-C
293	2-TricapCubeA_Mn_v4b_C2_g	-1625.51344590	66.52	C-C
294	3-OhfusetopentBipyr_Mn_v6a_C2_f	-1625.51191017	67.48	
295	3-OhfusetopentBipyr_Mn_v6b_C2_zb	-1625.51162131	67.66	
296	3-OhfusetopentBipyr_Mn_v6a_C2_q	-1625.51162124	67.66	
297	3-OhfusetopentBipyr_Mn_v5_C2_t	-1625.51162104	67.66	
298	3-OhfusetopentBipyr_Mn_v6b_C2_ze	-1625.51161826	67.67	
299	2-TricapCubeA_Mn_v4b_C2_f	-1625.51151167	67.73	C-C
300	4-Icos-1vx_Mn_v5a_C2_zj	-1625.51151165	67.73	C-C
301	4-Icos-1vx_Mn_v5b_C2_c	-1625.50964564	68.90	C-C
302	4-Icos-1vx_Mn_v5c_C2_x	-1625.50963356	68.91	C-C
303	4-Icos-1vx_Mn_v5a_C2_t	-1625.50962640	68.92	C-C
304	4-Icos-1vx_Mn_v5c_C2_g_r-284	-1625.50962607	68.92	C-C
305	4-Icos-1vx_Mn_v4_C2_m	-1625.50962593	68.92	C-C
306	3-OhfusetopentBipyr_Mn_v5_C2_u	-1625.50851249	69.62	
307	3-OhfusetopentBipyr_Mn_v6b_C2_j	-1625.50827343	69.77	
308	3-OhfusetopentBipyr_Mn_v5_C2_s	-1625.50775331	70.09	C-C
309	3-OhfusetopentBipyr_Mn_v6a_C2_p	-1625.50775320	70.09	
310	3-OhfusetopentBipyr_Mn_v5_C2_y	-1625.50719395	70.44	
311	3-OhfusetopentBipyr_Mn_v6b_C2_u	-1625.50704187	70.54	C-C
312	3-OhfusetopentBipyr_Mn_v5_C2_i	-1625.50704183	70.54	C-C
313	4-Icos-1vx_Mn_v5a_C2_zn	-1625.50568677	71.39	C-C
314	2-TricapCubeA_Mn_v4b_C2_v	-1625.50568136	71.39	C-C
315	3-OhfusetopentBipyr_Mn_v5_C2_c	-1625.50525241	71.66	
316	3-OhfusetopentBipyr_Mn_v4_C2_k	-1625.50525204	71.66	
317	3-OhfusetopentBipyr_Mn_v6b_C2_k	-1625.50525188	71.66	
318	3-OhfusetopentBipyr_Mn_v6b_C2_d	-1625.50522498	71.68	
319	4-Icos-1vx_Mn_v5a_C2_y	-1625.50519241	71.70	C-C
320	4-Icos-1vx_Mn_v4_C2_j	-1625.50440419	72.19	C-C
321	2-TricapCubeA_Mn_v4b_C2_d_r-31	-1625.50440416	72.19	C-C
322	4-Icos-1vx_Mn_v4_C2_w	-1625.50440267	72.19	C-C
323	4-Icos-1vx_Mn_v5b_C2_u_r-494 i-77	-1625.50434801	72.23	
324	2-TricapCubeA_Mn_v4b_C2_d	-1625.50341116	72.82	C-C
325	4-Icos-1vx_Mn_v5b_C2_n	-1625.50283926	73.18	C-C

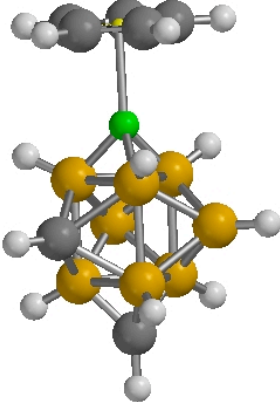
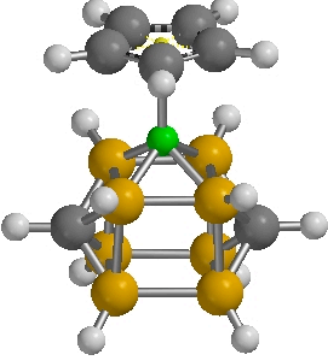
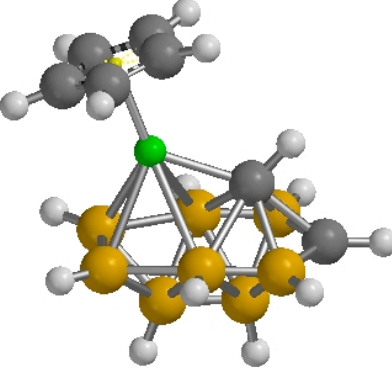
326	2-TricapCubeA_Mn_v4a_C2_v54g	-1625.50283779	73.18	C-C
327	4-Icos-1vx_Mn_v5b_C2_t	-1625.50263303	73.30	C-C
328	4-Icos-1vx_Mn_v5b_C2_p	-1625.50263279	73.30	C-C
329	2-TricapCubeB_Mn_v4_C2_t	-1625.50263185	73.31	C-C
330	3-OhfusetopentBipyr_Mn_v5_C2_w	-1625.50220388	73.57	C-C
331	4-Icos-1vx_Mn_v5c_C2_w i-204	-1625.50201867	73.69	
332	4-Icos-1vx_Mn_v5c_C2_b	-1625.50191279	73.76	C-C
333	4-Icos-1vx_Mn_v5c_C2_t	-1625.50191159	73.76	
334	3-OhfusetopentBipyr_Mn_v5_C2_j	-1625.50127036	74.16	
335	4-Icos-1vx_Mn_v5c_C2_z	-1625.50126314	74.16	C-C
336	2-TricapCubeA_Mn_v4b_C2_r	-1625.50126269	74.16	C-C
337	3-OhfusetopentBipyr_Mn_v6a_C2_d	-1625.50104107	74.30	C-C
338	3-OhfusetopentBipyr_Mn_v5_C2_h r-16	-1625.50102233	74.32	C-C
339	3-OhfusetopentBipyr_Mn_v6a_C2_g	-1625.50084822	74.42	C-C
340	3-OhfusetopentBipyr_Mn_v5_C2_h i-16	-1625.50056770	74.60	C-C
341	2-TricapCubeB_Mn_v6_C2_s	-1625.50044517	74.68	C-C
342	1-PentaCapTrPr_Mn_v3_C2_v63b	-1625.49997864	74.97	C-C
343	2-TricapCubeB_Mn_v6_C2_p	-1625.49997723	74.97	C-C
344	3-OhfusetopentBipyr_Mn_v4_C2_b	-1625.49934405	75.37	
345	1-PentaCapTrPr_Mn_v3_C2_v64c	-1625.49856589	75.86	C-C
346	4-Icos-1vx_Mn_v4_C2_g	-1625.49674045	77.00	C-C
347	4-Icos-1vx_Mn_v4_C2_n	-1625.49674018	77.00	C-C
348	1-PentaCapTrPr_Mn_v4_C2_v64c	-1625.49673179	77.01	C-C
349	4-Icos-1vx_Mn_v5b_C2_u i-494	-1625.49637520	77.23	
350	4-Icos-1vx_Mn_v5a_C2_r	-1625.49610472	77.40	C-C
351	4-Icos-1vx_Mn_v4_C2_s	-1625.49610144	77.40	C-C
352	3-OhfusetopentBipyr_Mn_v4_C2_j	-1625.49568041	77.67	
353	3-OhfusetopentBipyr_Mn_v4_C2_v	-1625.49451942	78.40	C-C
354	3-OhfusetopentBipyr_Mn_v6a_C2_j	-1625.49389752	78.79	
355	3-OhfusetopentBipyr_Mn_v4_C2_i	-1625.49267103	79.56	
356	3-OhfusetopentBipyr_Mn_v4_C2_q	-1625.49195195	80.01	
357	3-OhfusetopentBipyr_Mn_v6b_C2_m	-1625.49134960	80.39	C-C
358	3-OhfusetopentBipyr_Mn_v6b_C2_x	-1625.49134943	80.39	
359	3-OhfusetopentBipyr_Mn_v5_C2_r	-1625.49011060	81.16	C-C
360	4-Icos-1vx_Mn_v5c_C2_q	-1625.48997303	81.25	C-C
361	3-OhfusetopentBipyr_Mn_v6b_C2_z	-1625.48988947	81.30	
362	4-Icos-1vx_Mn_v5b_C2_j r-148	-1625.48840705	82.23	C-C
363	4-Icos-1vx_Mn_v5c_C2_zz i-262	-1625.48798729	82.49	
364	3-OhfusetopentBipyr_Mn_v5_C2_z	-1625.48704688	83.09	
365	4-Icos-1vx_Mn_v5a_C2_za	-1625.48699573	83.12	C-C
366	3-OhfusetopentBipyr_Mn_v5_C2_e	-1625.48544505	84.09	

367	4-Icos-1vx_Mn_v5b_C2_x	-1625.48413371	84.91	C-C
368	1-PentaCapTrPr_Mn_v4_C2_v66f	-1625.48393254	85.04	C-C
369	3-OhfusetopentBipyr_Mn_v6b_C2_o	-1625.48369341	85.19	
370	3-OhfusetopentBipyr_Mn_v6b_C2_i	-1625.48353746	85.29	
371	4-Icos-1vx_Mn_v5b_C2_j i-148	-1625.48332710	85.42	C-C
372	4-Icos-1vx_Mn_v5c_C2_l	-1625.48301555	85.61	C-C
373	3-OhfusetopentBipyr_Mn_v6a_C2_k	-1625.48301155	85.62	
374	3-OhfusetopentBipyr_Mn_v5_C2_n	-1625.48300996	85.62	
375	3-OhfusetopentBipyr_Mn_v6b_C2_n	-1625.48287838	85.70	C-C
376	3-OhfusetopentBipyr_Mn_v4_C2_r	-1625.48181101	86.37	C-C
377	3-OhfusetopentBipyr_Mn_v6b_C2_y	-1625.48171372	86.43	
378	3-OhfusetopentBipyr_Mn_v4_C2_f r-22	-1625.47999829	87.51	C-C
379	4-Icos-1vx_Mn_v5b_C2_g	-1625.47894367	88.17	
380	3-OhfusetopentBipyr_Mn_v4_C2_f i-22	-1625.47890735	88.19	C-C
381	3-OhfusetopentBipyr_Mn_v5_C2_a	-1625.47876532	88.28	C-C
382	2-TricapCubeA_Mn_v4b_C2_y	-1625.47746898	89.10	C-C
383	3-OhfusetopentBipyr_Mn_v6b_C2_c	-1625.47707843	89.34	
384	3-OhfusetopentBipyr_Mn_v6b_C2_p	-1625.47707793	89.34	
385	3-OhfusetopentBipyr_Mn_v6b_C2_a	-1625.47591829	90.07	C-C
386	3-OhfusetopentBipyr_Mn_v4_C2_w	-1625.47591792	90.07	C-C
387	3-OhfusetopentBipyr_Mn_v6b_C2_w	-1625.47591716	90.07	C-C
388	3-OhfusetopentBipyr_Mn_v6a_C2_w	-1625.47581540	90.13	C-C
389	4-Icos-1vx_Mn_v5b_C2_a imag	-1625.47474159	90.81	
390	3-OhfusetopentBipyr_Mn_v4_C2_n	-1625.47146782	92.86	C-C
391	3-OhfusetopentBipyr_Mn_v6b_C2_e	-1625.47005447	93.75	
392	3-OhfusetopentBipyr_Mn_v6a_C2_z	-1625.46857938	94.67	C-C
393	3-OhfusetopentBipyr_Mn_v5_C2_x	-1625.46857925	94.67	C-C
394	3-OhfusetopentBipyr_Mn_v4_C2_h	-1625.46738100	95.43	C-C
395	3-OhfusetopentBipyr_Mn_v5_C2_o	-1625.46532330	96.72	C-C
396	4-Icos-1vx_Mn_v5c_C2_g r-284	-1625.46486323	97.01	C-C
397	3-OhfusetopentBipyr_Mn_v6a_C2_h i-13	-1625.46368253	97.75	
398	1-PentaCapTrPr_Mn_v3_C2_v66b	-1625.46129374	99.25	
399	4-Icos-1vx_Mn_v5c_C2_p	-1625.46027276	99.89	C-C
400	3-OhfusetopentBipyr_Mn_v6a_C2_i	-1625.45878265	100.82	C-C
401	3-OhfusetopentBipyr_Mn_v6b_C2_s	-1625.45739684	101.69	
402	3-OhfusetopentBipyr_Mn_v6b_C2_h	-1625.45739649	101.69	C-C
403	3-OhfusetopentBipyr_Mn_v5_C2_q	-1625.45380207	103.95	C-C
404	3-OhfusetopentBipyr_Mn_v6a_C2_o	-1625.45380093	103.95	C-C
405	3-OhfusetopentBipyr_Mn_v5_C2_b	-1625.45335041	104.23	
406	3-OhfusetopentBipyr_Mn_v4_C2_a	-1625.45304790	104.42	C-C
407	3-OhfusetopentBipyr_Mn_v4_C2_e r-19-13	-1625.44672732	108.39	

408	3-OhfusettoPentBipyr_Mn_v4_C2_e_r-19	-1625.44672731	108.39	
409	3-OhfusettoPentBipyr_Mn_v4_C2_e_i-19	-1625.44671041	108.40	
410	3-OhfusettoPentBipyr_Mn_v6b_C2_zd	-1625.44615665	108.74	
411	3-OhfusettoPentBipyr_Mn_v6a_C2_s	-1625.44476674	109.62	C-C
412	3-OhfusettoPentBipyr_Mn_v6b_C2_zc	-1625.43118290	118.14	
413	3-OhfusettoPentBipyr_Mn_v4_C2_o	-1625.43050178	118.57	
414	4-Icos-1vx_Mn_v5c_C2_h_imag	-1625.41836739	126.18	
415	3-OhfusettoPentBipyr_Mn_v4_C2_s	-1625.40569864	134.13	C-C
416	3-OhfusettoPentBipyr_Mn_v6a_C2_a	-1625.40260347	136.07	C-C

11-vertex $\text{CpReC}_2\text{B}_8\text{H}_{10}$

Table 1. Initial structures (one example from each family) 389 structures in total

Initial structures
 <p>1. Pentacapped trigonal prism 49 structures</p>
 <p>2. Tricapped cube 94 structures</p>
 <p>3. Octahedron fused to pentagonal bipyramid 108 structures</p>

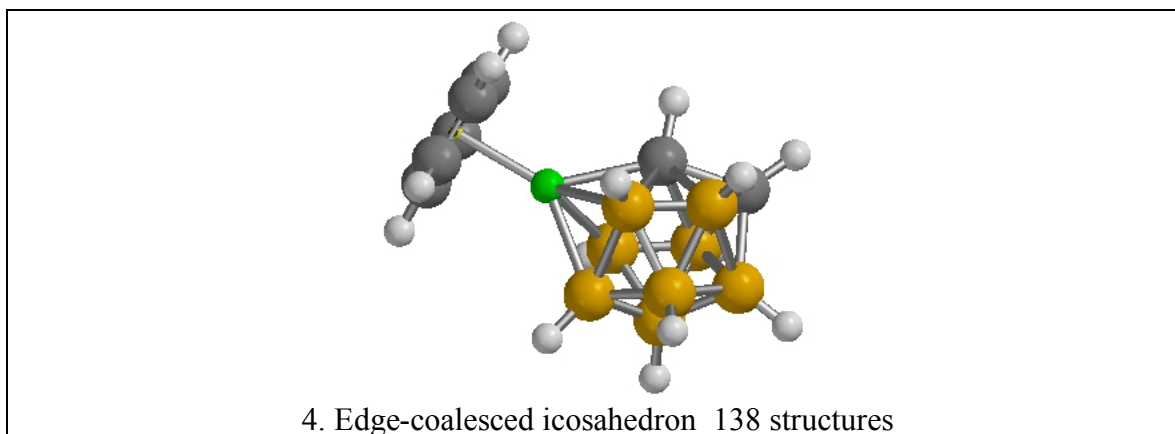
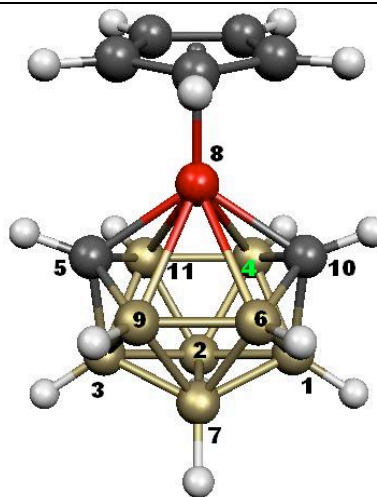
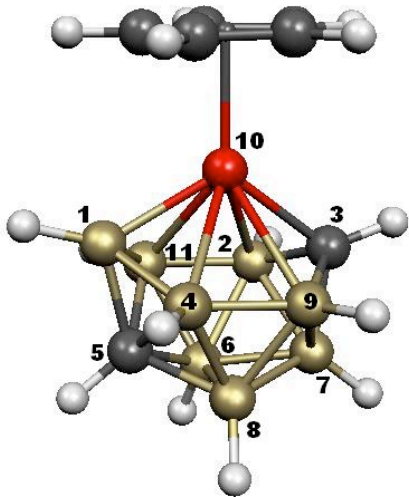
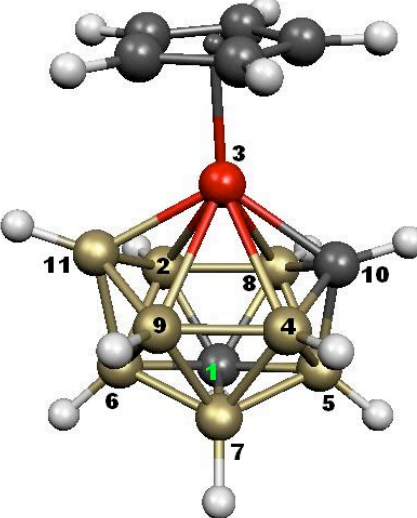
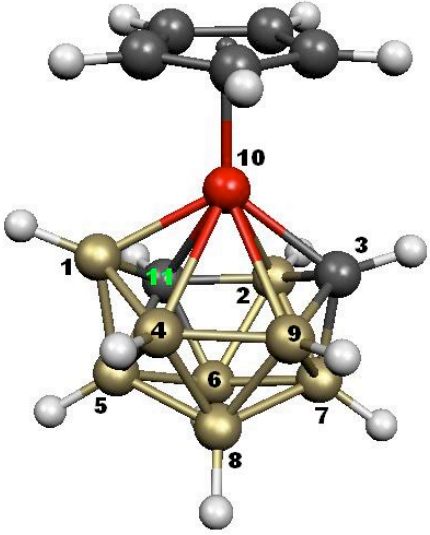
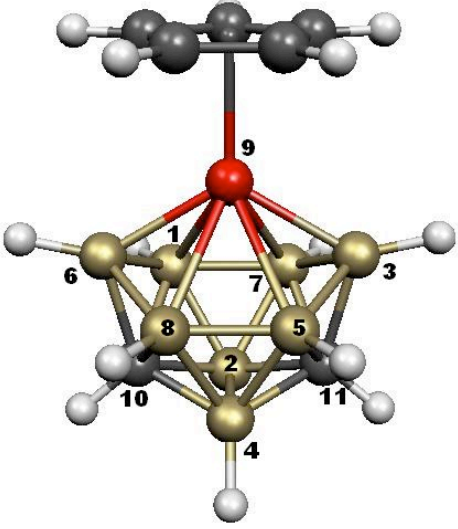


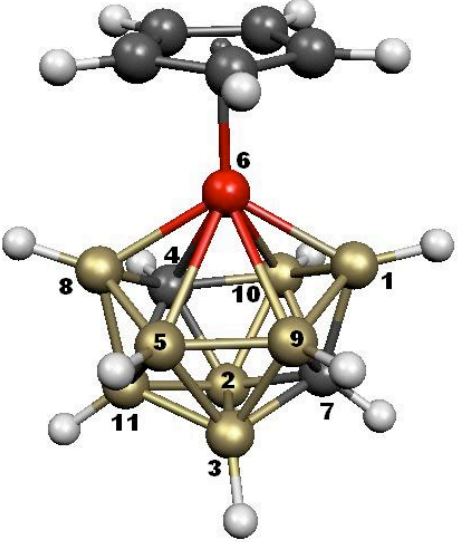
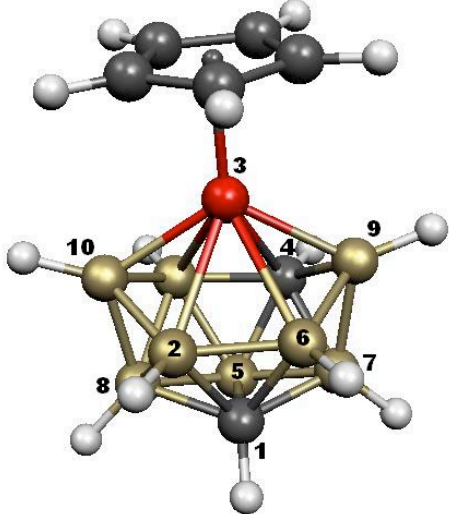
Table 3. Distances table for the best structures

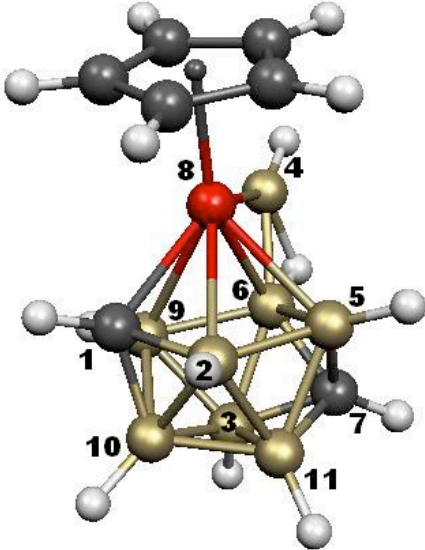
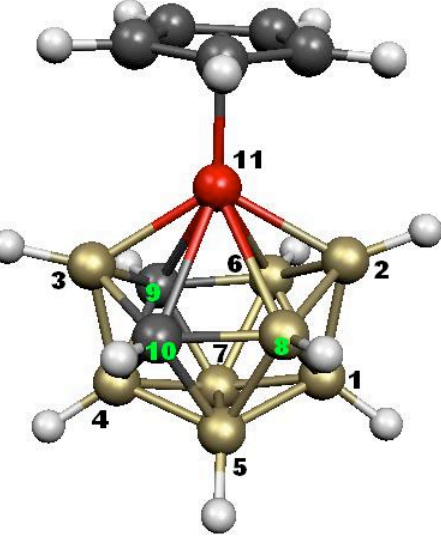
		1	2	3	4	5	
	1 B	0.000000					
	2 B	1.780510	0.000000				
	3 B	2.974800	1.780510	0.000000			
	4 B	1.853399	1.813993	2.951674	0.000000		
	5 C	3.536422	2.765295	1.631403	2.929705	0.000000	
	6 B	1.853389	2.853079	2.951366	2.723103	2.929176	
	7 B	1.779714	1.779303	1.779714	2.852146	2.765046	
	8 Re	3.165866	3.320877	3.165866	2.341798	2.027657	
	9 B	2.951366	2.853079	1.853389	3.249816	1.646567	
	10 C	1.631403	2.765295	3.536422	1.646906	3.309400	
11 B	2.951674	1.813993	1.853399	1.774000	1.646906		
		6	7	8	9	10	
6 B	0.000000						
7 B	1.814876	0.000000					
8 Re	2.346949	3.323495	0.000000				
9 B	1.773400	1.814876	2.346949	0.000000			
10 C	1.646567	2.765046	2.027657	2.929176	0.000000		
11 B	3.249816	2.852146	2.341798	2.723103	2.929705		

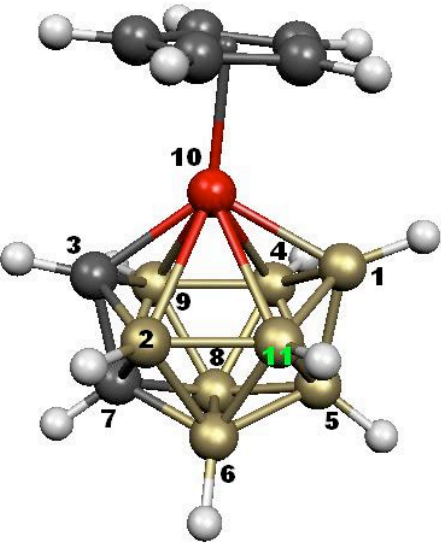
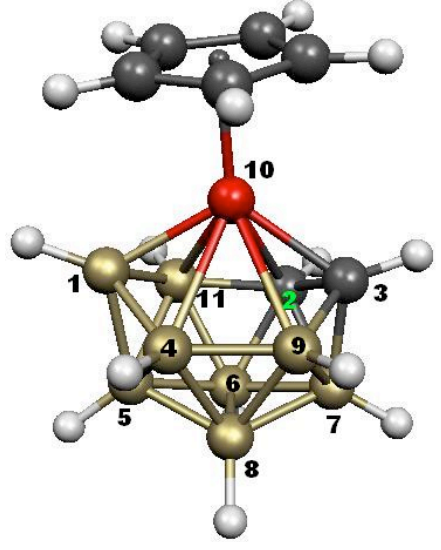
1. -553.04867037 0.0 kcal/mole Cs

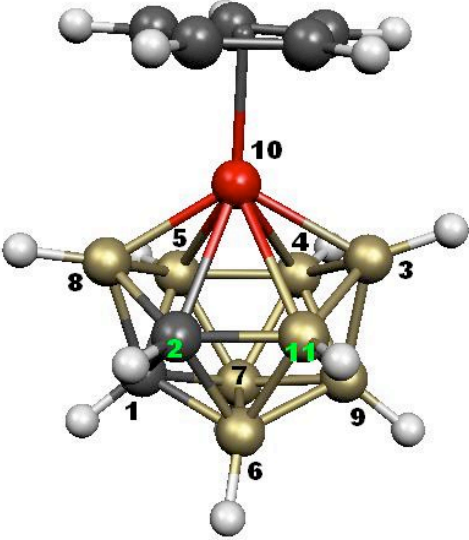
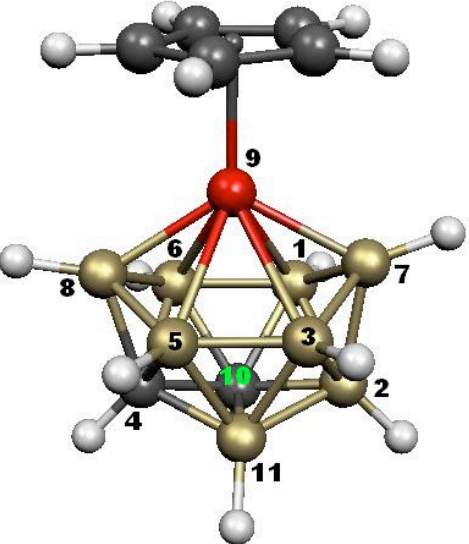
 <p>2. -553.04465894 +2.5 Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.088715</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>3.450917</td><td>1.639243</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.760931</td><td>3.234597</td><td>2.892013</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>1.692150</td><td>2.809889</td><td>3.357462</td><td>1.761881</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.924724</td><td>1.811550</td><td>2.755038</td><td>2.839259</td><td>1.686666</td></tr> <tr><td>7 B</td><td>3.713273</td><td>1.850546</td><td>1.634030</td><td>2.925544</td><td>2.829367</td></tr> <tr><td>8 B</td><td>2.924068</td><td>2.852474</td><td>2.755110</td><td>1.798395</td><td>1.686035</td></tr> <tr><td>9 B</td><td>3.087470</td><td>2.725003</td><td>1.639422</td><td>1.754790</td><td>2.809446</td></tr> <tr><td>10 Re</td><td>2.073830</td><td>2.360850</td><td>2.045865</td><td>2.318404</td><td>3.004964</td></tr> <tr><td>11 B</td><td>1.761651</td><td>1.755080</td><td>2.891360</td><td>2.707703</td><td>1.761035</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.775809</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.781703</td><td>1.774948</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.852892</td><td>1.849896</td><td>1.812071</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.316858</td><td>3.183044</td><td>3.319647</td><td>2.366304</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.797241</td><td>2.925288</td><td>2.837525</td><td>3.233261</td><td>2.312072</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.088715	0.000000				3 C	3.450917	1.639243	0.000000			4 B	1.760931	3.234597	2.892013	0.000000		5 C	1.692150	2.809889	3.357462	1.761881	0.000000	6 B	2.924724	1.811550	2.755038	2.839259	1.686666	7 B	3.713273	1.850546	1.634030	2.925544	2.829367	8 B	2.924068	2.852474	2.755110	1.798395	1.686035	9 B	3.087470	2.725003	1.639422	1.754790	2.809446	10 Re	2.073830	2.360850	2.045865	2.318404	3.004964	11 B	1.761651	1.755080	2.891360	2.707703	1.761035		6	7	8	9	10	6 B	0.000000					7 B	1.775809	0.000000				8 B	1.781703	1.774948	0.000000			9 B	2.852892	1.849896	1.812071	0.000000		10 Re	3.316858	3.183044	3.319647	2.366304	0.000000	11 B	1.797241	2.925288	2.837525	3.233261	2.312072
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	3.088715	0.000000																																																																																																																	
3 C	3.450917	1.639243	0.000000																																																																																																																
4 B	1.760931	3.234597	2.892013	0.000000																																																																																																															
5 C	1.692150	2.809889	3.357462	1.761881	0.000000																																																																																																														
6 B	2.924724	1.811550	2.755038	2.839259	1.686666																																																																																																														
7 B	3.713273	1.850546	1.634030	2.925544	2.829367																																																																																																														
8 B	2.924068	2.852474	2.755110	1.798395	1.686035																																																																																																														
9 B	3.087470	2.725003	1.639422	1.754790	2.809446																																																																																																														
10 Re	2.073830	2.360850	2.045865	2.318404	3.004964																																																																																																														
11 B	1.761651	1.755080	2.891360	2.707703	1.761035																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.775809	0.000000																																																																																																																	
8 B	1.781703	1.774948	0.000000																																																																																																																
9 B	2.852892	1.849896	1.812071	0.000000																																																																																																															
10 Re	3.316858	3.183044	3.319647	2.366304	0.000000																																																																																																														
11 B	1.797241	2.925288	2.837525	3.233261	2.312072																																																																																																														
 <p>3. -553.03906771 +6.0</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.724466</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>3.173108</td><td>2.324206</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.711184</td><td>3.232061</td><td>2.355178</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.698309</td><td>2.917140</td><td>3.156825</td><td>1.839006</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.690923</td><td>1.827856</td><td>3.139600</td><td>2.937635</td><td>2.940297</td></tr> <tr><td>7 B</td><td>1.695722</td><td>2.832590</td><td>3.313551</td><td>1.807140</td><td>1.777152</td></tr> <tr><td>8 B</td><td>1.750287</td><td>1.757352</td><td>2.324721</td><td>2.711159</td><td>1.848196</td></tr> <tr><td>9 B</td><td>2.698557</td><td>2.699966</td><td>2.338302</td><td>1.771793</td><td>2.923524</td></tr> <tr><td>10 C</td><td>2.645549</td><td>2.913987</td><td>2.044372</td><td>1.651276</td><td>1.624146</td></tr> <tr><td>11 B</td><td>2.824742</td><td>1.752830</td><td>2.083896</td><td>3.100328</td><td>3.714001</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.764262</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.929226</td><td>2.856019</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.837288</td><td>1.787613</td><td>3.228130</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>3.519344</td><td>2.768916</td><td>1.630989</td><td>2.928121</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.764365</td><td>2.940803</td><td>3.073125</td><td>1.774947</td><td>3.475889</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.724466	0.000000				3 Re	3.173108	2.324206	0.000000			4 B	2.711184	3.232061	2.355178	0.000000		5 B	1.698309	2.917140	3.156825	1.839006	0.000000	6 B	1.690923	1.827856	3.139600	2.937635	2.940297	7 B	1.695722	2.832590	3.313551	1.807140	1.777152	8 B	1.750287	1.757352	2.324721	2.711159	1.848196	9 B	2.698557	2.699966	2.338302	1.771793	2.923524	10 C	2.645549	2.913987	2.044372	1.651276	1.624146	11 B	2.824742	1.752830	2.083896	3.100328	3.714001		6	7	8	9	10	6 B	0.000000					7 B	1.764262	0.000000				8 B	2.929226	2.856019	0.000000			9 B	1.837288	1.787613	3.228130	0.000000		10 C	3.519344	2.768916	1.630989	2.928121	0.000000	11 B	1.764365	2.940803	3.073125	1.774947	3.475889
	1	2	3	4	5																																																																																																														
1 C	0.000000																																																																																																																		
2 B	1.724466	0.000000																																																																																																																	
3 Re	3.173108	2.324206	0.000000																																																																																																																
4 B	2.711184	3.232061	2.355178	0.000000																																																																																																															
5 B	1.698309	2.917140	3.156825	1.839006	0.000000																																																																																																														
6 B	1.690923	1.827856	3.139600	2.937635	2.940297																																																																																																														
7 B	1.695722	2.832590	3.313551	1.807140	1.777152																																																																																																														
8 B	1.750287	1.757352	2.324721	2.711159	1.848196																																																																																																														
9 B	2.698557	2.699966	2.338302	1.771793	2.923524																																																																																																														
10 C	2.645549	2.913987	2.044372	1.651276	1.624146																																																																																																														
11 B	2.824742	1.752830	2.083896	3.100328	3.714001																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.764262	0.000000																																																																																																																	
8 B	2.929226	2.856019	0.000000																																																																																																																
9 B	1.837288	1.787613	3.228130	0.000000																																																																																																															
10 C	3.519344	2.768916	1.630989	2.928121	0.000000																																																																																																														
11 B	1.764365	2.940803	3.073125	1.774947	3.475889																																																																																																														

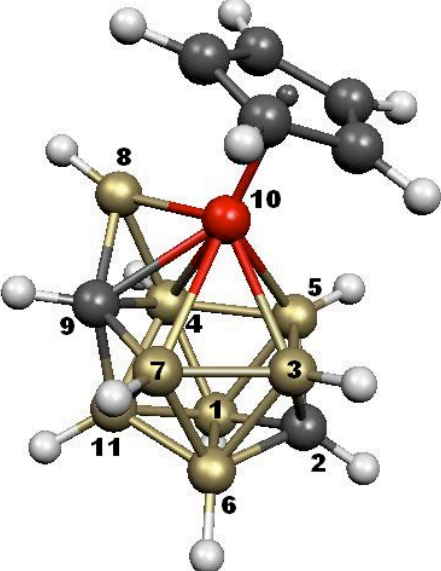
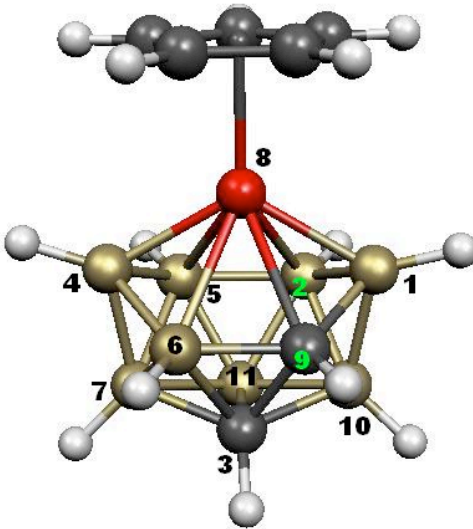
 <p>4. -553.03654077 +7.6</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.015866</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>3.429354</td><td>1.650866</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.762023</td><td>3.232932</td><td>2.925475</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.755324</td><td>2.919615</td><td>3.505319</td><td>1.828393</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.912498</td><td>1.837640</td><td>2.769548</td><td>2.842269</td><td>1.755582</td></tr> <tr><td>7 B</td><td>3.695223</td><td>1.861381</td><td>1.623832</td><td>2.958421</td><td>2.950643</td></tr> <tr><td>8 B</td><td>2.937392</td><td>2.861206</td><td>2.765169</td><td>1.821198</td><td>1.760702</td></tr> <tr><td>9 B</td><td>3.070740</td><td>2.720878</td><td>1.647313</td><td>1.774871</td><td>2.914236</td></tr> <tr><td>10 Re</td><td>2.075487</td><td>2.331304</td><td>2.032187</td><td>2.346618</td><td>3.157114</td></tr> <tr><td>11 C</td><td>1.686666</td><td>1.671542</td><td>2.803758</td><td>2.587370</td><td>1.749904</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.775330</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.766530</td><td>1.791123</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.837693</td><td>1.851722</td><td>1.802929</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.343365</td><td>3.172367</td><td>3.338693</td><td>2.357792</td><td>0.000000</td></tr> <tr><td>11 C</td><td>1.712704</td><td>2.798693</td><td>2.702793</td><td>3.090601</td><td>2.290250</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.015866	0.000000				3 C	3.429354	1.650866	0.000000			4 B	1.762023	3.232932	2.925475	0.000000		5 B	1.755324	2.919615	3.505319	1.828393	0.000000	6 B	2.912498	1.837640	2.769548	2.842269	1.755582	7 B	3.695223	1.861381	1.623832	2.958421	2.950643	8 B	2.937392	2.861206	2.765169	1.821198	1.760702	9 B	3.070740	2.720878	1.647313	1.774871	2.914236	10 Re	2.075487	2.331304	2.032187	2.346618	3.157114	11 C	1.686666	1.671542	2.803758	2.587370	1.749904		6	7	8	9	10	6 B	0.000000					7 B	1.775330	0.000000				8 B	1.766530	1.791123	0.000000			9 B	2.837693	1.851722	1.802929	0.000000		10 Re	3.343365	3.172367	3.338693	2.357792	0.000000	11 C	1.712704	2.798693	2.702793	3.090601	2.290250
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	3.015866	0.000000																																																																																																																	
3 C	3.429354	1.650866	0.000000																																																																																																																
4 B	1.762023	3.232932	2.925475	0.000000																																																																																																															
5 B	1.755324	2.919615	3.505319	1.828393	0.000000																																																																																																														
6 B	2.912498	1.837640	2.769548	2.842269	1.755582																																																																																																														
7 B	3.695223	1.861381	1.623832	2.958421	2.950643																																																																																																														
8 B	2.937392	2.861206	2.765169	1.821198	1.760702																																																																																																														
9 B	3.070740	2.720878	1.647313	1.774871	2.914236																																																																																																														
10 Re	2.075487	2.331304	2.032187	2.346618	3.157114																																																																																																														
11 C	1.686666	1.671542	2.803758	2.587370	1.749904																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.775330	0.000000																																																																																																																	
8 B	1.766530	1.791123	0.000000																																																																																																																
9 B	2.837693	1.851722	1.802929	0.000000																																																																																																															
10 Re	3.343365	3.172367	3.338693	2.357792	0.000000																																																																																																														
11 C	1.712704	2.798693	2.702793	3.090601	2.290250																																																																																																														
 <p>5. -553.02844903 +12.7 Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.786477</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.053425</td><td>2.903909</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.843182</td><td>1.797005</td><td>2.904285</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.231625</td><td>2.842055</td><td>1.753644</td><td>1.785695</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.753199</td><td>2.903909</td><td>3.585600</td><td>2.904285</td><td>3.053446</td></tr> <tr><td>7 B</td><td>1.743000</td><td>1.786477</td><td>1.753199</td><td>2.843182</td><td>2.721406</td></tr> <tr><td>8 B</td><td>2.721406</td><td>2.842055</td><td>3.053446</td><td>1.785695</td><td>1.742600</td></tr> <tr><td>9 Re</td><td>2.339109</td><td>3.301573</td><td>2.090246</td><td>3.298281</td><td>2.331773</td></tr> <tr><td>10 C</td><td>1.765155</td><td>1.681452</td><td>3.534763</td><td>1.682128</td><td>2.791802</td></tr> <tr><td>11 C</td><td>2.792020</td><td>1.681452</td><td>1.693496</td><td>1.682128</td><td>1.765113</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.053425</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.753644</td><td>3.231625</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Re</td><td>2.090246</td><td>2.339109</td><td>2.331773</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>1.693496</td><td>2.792020</td><td>1.765113</td><td>3.021749</td><td>0.000000</td></tr> <tr><td>11 C</td><td>3.534763</td><td>1.765155</td><td>2.791802</td><td>3.021749</td><td>2.684800</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.786477	0.000000				3 B	3.053425	2.903909	0.000000			4 B	2.843182	1.797005	2.904285	0.000000		5 B	3.231625	2.842055	1.753644	1.785695	0.000000	6 B	1.753199	2.903909	3.585600	2.904285	3.053446	7 B	1.743000	1.786477	1.753199	2.843182	2.721406	8 B	2.721406	2.842055	3.053446	1.785695	1.742600	9 Re	2.339109	3.301573	2.090246	3.298281	2.331773	10 C	1.765155	1.681452	3.534763	1.682128	2.791802	11 C	2.792020	1.681452	1.693496	1.682128	1.765113		6	7	8	9	10	6 B	0.000000					7 B	3.053425	0.000000				8 B	1.753644	3.231625	0.000000			9 Re	2.090246	2.339109	2.331773	0.000000		10 C	1.693496	2.792020	1.765113	3.021749	0.000000	11 C	3.534763	1.765155	2.791802	3.021749	2.684800
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.786477	0.000000																																																																																																																	
3 B	3.053425	2.903909	0.000000																																																																																																																
4 B	2.843182	1.797005	2.904285	0.000000																																																																																																															
5 B	3.231625	2.842055	1.753644	1.785695	0.000000																																																																																																														
6 B	1.753199	2.903909	3.585600	2.904285	3.053446																																																																																																														
7 B	1.743000	1.786477	1.753199	2.843182	2.721406																																																																																																														
8 B	2.721406	2.842055	3.053446	1.785695	1.742600																																																																																																														
9 Re	2.339109	3.301573	2.090246	3.298281	2.331773																																																																																																														
10 C	1.765155	1.681452	3.534763	1.682128	2.791802																																																																																																														
11 C	2.792020	1.681452	1.693496	1.682128	1.765113																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	3.053425	0.000000																																																																																																																	
8 B	1.753644	3.231625	0.000000																																																																																																																
9 Re	2.090246	2.339109	2.331773	0.000000																																																																																																															
10 C	1.693496	2.792020	1.765113	3.021749	0.000000																																																																																																														
11 C	3.534763	1.765155	2.791802	3.021749	2.684800																																																																																																														

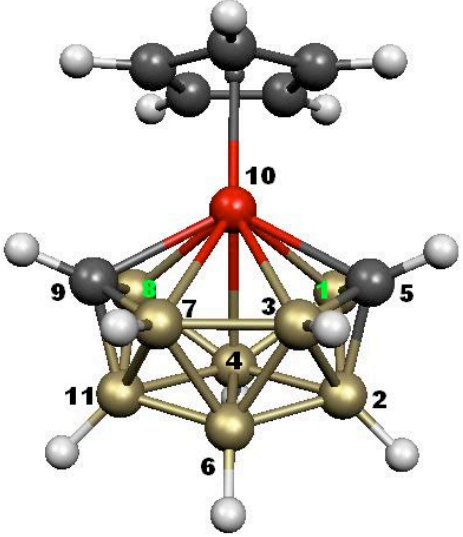
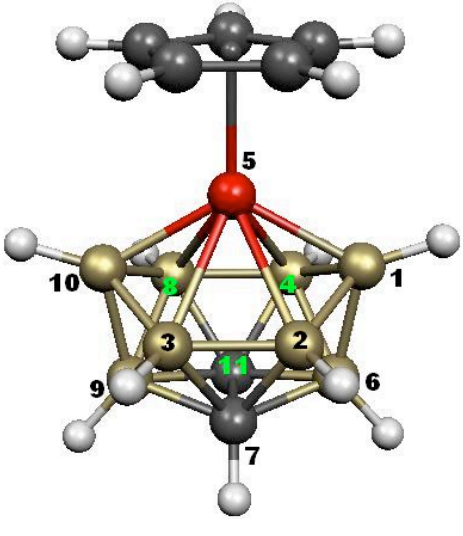
 <p>6. -553.02671402 +13.8</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.917378</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.915567</td><td>1.765653</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>2.971190</td><td>1.710122</td><td>2.708144</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.086059</td><td>2.834457</td><td>1.811690</td><td>2.596394</td><td>0.000000</td></tr> <tr><td>6 Re</td><td>2.080794</td><td>3.326361</td><td>3.329897</td><td>2.304359</td><td>2.373611</td></tr> <tr><td>7 C</td><td>1.676495</td><td>1.673539</td><td>1.702776</td><td>2.658972</td><td>2.821910</td></tr> <tr><td>8 B</td><td>3.566960</td><td>2.894907</td><td>2.919922</td><td>1.679842</td><td>1.750431</td></tr> <tr><td>9 B</td><td>1.755784</td><td>2.820899</td><td>1.790472</td><td>3.080333</td><td>1.755658</td></tr> <tr><td>10 B</td><td>1.765525</td><td>1.832325</td><td>2.860537</td><td>1.657620</td><td>3.226133</td></tr> <tr><td>11 B</td><td>3.684534</td><td>1.751514</td><td>1.759526</td><td>1.752714</td><td>1.825324</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 C</td><td>3.009430</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.092481</td><td>3.514598</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.322139</td><td>1.773323</td><td>3.024257</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.288118</td><td>1.777162</td><td>2.978564</td><td>2.712456</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.174877</td><td>2.811538</td><td>1.754893</td><td>2.895004</td><td>2.908518</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.917378	0.000000				3 B	2.915567	1.765653	0.000000			4 C	2.971190	1.710122	2.708144	0.000000		5 B	3.086059	2.834457	1.811690	2.596394	0.000000	6 Re	2.080794	3.326361	3.329897	2.304359	2.373611	7 C	1.676495	1.673539	1.702776	2.658972	2.821910	8 B	3.566960	2.894907	2.919922	1.679842	1.750431	9 B	1.755784	2.820899	1.790472	3.080333	1.755658	10 B	1.765525	1.832325	2.860537	1.657620	3.226133	11 B	3.684534	1.751514	1.759526	1.752714	1.825324		6	7	8	9	10	6 Re	0.000000					7 C	3.009430	0.000000				8 B	2.092481	3.514598	0.000000			9 B	2.322139	1.773323	3.024257	0.000000		10 B	2.288118	1.777162	2.978564	2.712456	0.000000	11 B	3.174877	2.811538	1.754893	2.895004	2.908518
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	2.917378	0.000000																																																																																																																	
3 B	2.915567	1.765653	0.000000																																																																																																																
4 C	2.971190	1.710122	2.708144	0.000000																																																																																																															
5 B	3.086059	2.834457	1.811690	2.596394	0.000000																																																																																																														
6 Re	2.080794	3.326361	3.329897	2.304359	2.373611																																																																																																														
7 C	1.676495	1.673539	1.702776	2.658972	2.821910																																																																																																														
8 B	3.566960	2.894907	2.919922	1.679842	1.750431																																																																																																														
9 B	1.755784	2.820899	1.790472	3.080333	1.755658																																																																																																														
10 B	1.765525	1.832325	2.860537	1.657620	3.226133																																																																																																														
11 B	3.684534	1.751514	1.759526	1.752714	1.825324																																																																																																														
	6	7	8	9	10																																																																																																														
6 Re	0.000000																																																																																																																		
7 C	3.009430	0.000000																																																																																																																	
8 B	2.092481	3.514598	0.000000																																																																																																																
9 B	2.322139	1.773323	3.024257	0.000000																																																																																																															
10 B	2.288118	1.777162	2.978564	2.712456	0.000000																																																																																																														
11 B	3.174877	2.811538	1.754893	2.895004	2.908518																																																																																																														
 <p>7. -553.02262146 +16.4</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.721462</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>3.182677</td><td>2.327248</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>2.560799</td><td>3.077421</td><td>2.296628</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.679756</td><td>2.812064</td><td>3.315552</td><td>1.703896</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.758875</td><td>1.770169</td><td>2.333490</td><td>2.580641</td><td>2.845965</td></tr> <tr><td>7 B</td><td>1.680579</td><td>2.884735</td><td>3.141674</td><td>1.742539</td><td>1.775737</td></tr> <tr><td>8 B</td><td>1.703074</td><td>1.829711</td><td>3.141355</td><td>2.795111</td><td>1.752224</td></tr> <tr><td>9 B</td><td>2.811791</td><td>3.051266</td><td>2.092346</td><td>1.687673</td><td>2.909967</td></tr> <tr><td>10 B</td><td>2.712011</td><td>2.703937</td><td>2.322788</td><td>1.678606</td><td>1.800462</td></tr> <tr><td>11 B</td><td>2.818384</td><td>1.745497</td><td>2.087099</td><td>2.983890</td><td>2.925185</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.810239</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.946599</td><td>2.932007</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.740955</td><td>1.735592</td><td>3.678757</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.227607</td><td>2.910428</td><td>1.853592</td><td>3.019944</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.079027</td><td>3.686661</td><td>1.747977</td><td>3.591647</td><td>1.781720</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.721462	0.000000				3 Re	3.182677	2.327248	0.000000			4 C	2.560799	3.077421	2.296628	0.000000		5 B	1.679756	2.812064	3.315552	1.703896	0.000000	6 B	1.758875	1.770169	2.333490	2.580641	2.845965	7 B	1.680579	2.884735	3.141674	1.742539	1.775737	8 B	1.703074	1.829711	3.141355	2.795111	1.752224	9 B	2.811791	3.051266	2.092346	1.687673	2.909967	10 B	2.712011	2.703937	2.322788	1.678606	1.800462	11 B	2.818384	1.745497	2.087099	2.983890	2.925185		6	7	8	9	10	6 B	0.000000					7 B	1.810239	0.000000				8 B	2.946599	2.932007	0.000000			9 B	1.740955	1.735592	3.678757	0.000000		10 B	3.227607	2.910428	1.853592	3.019944	0.000000	11 B	3.079027	3.686661	1.747977	3.591647	1.781720
	1	2	3	4	5																																																																																																														
1 C	0.000000																																																																																																																		
2 B	1.721462	0.000000																																																																																																																	
3 Re	3.182677	2.327248	0.000000																																																																																																																
4 C	2.560799	3.077421	2.296628	0.000000																																																																																																															
5 B	1.679756	2.812064	3.315552	1.703896	0.000000																																																																																																														
6 B	1.758875	1.770169	2.333490	2.580641	2.845965																																																																																																														
7 B	1.680579	2.884735	3.141674	1.742539	1.775737																																																																																																														
8 B	1.703074	1.829711	3.141355	2.795111	1.752224																																																																																																														
9 B	2.811791	3.051266	2.092346	1.687673	2.909967																																																																																																														
10 B	2.712011	2.703937	2.322788	1.678606	1.800462																																																																																																														
11 B	2.818384	1.745497	2.087099	2.983890	2.925185																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.810239	0.000000																																																																																																																	
8 B	2.946599	2.932007	0.000000																																																																																																																
9 B	1.740955	1.735592	3.678757	0.000000																																																																																																															
10 B	3.227607	2.910428	1.853592	3.019944	0.000000																																																																																																														
11 B	3.079027	3.686661	1.747977	3.591647	1.781720																																																																																																														

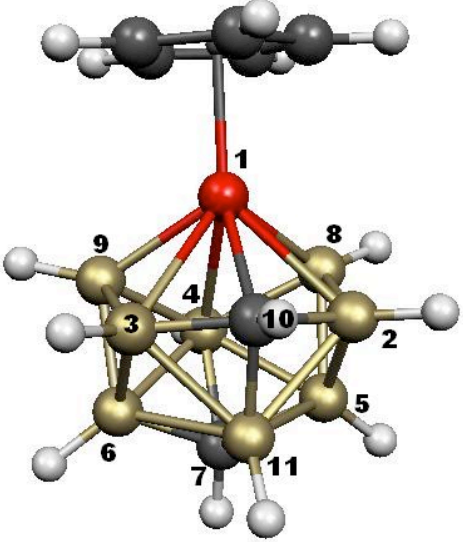
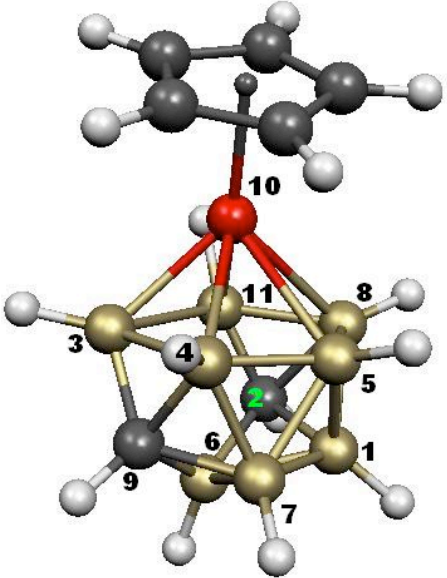
 <p>8. -553.02085934 +17.5</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.638447</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.751430</td><td>2.830220</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.540311</td><td>3.896820</td><td>3.464098</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.881986</td><td>1.815108</td><td>2.702647</td><td>3.033995</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.754619</td><td>2.811602</td><td>1.829719</td><td>1.722740</td><td>1.959926</td></tr> <tr><td>7 C</td><td>3.386131</td><td>2.749772</td><td>1.637665</td><td>3.178848</td><td>1.628390</td></tr> <tr><td>8 Re</td><td>2.124482</td><td>2.381084</td><td>3.465957</td><td>2.029992</td><td>2.306030</td></tr> <tr><td>9 B</td><td>1.601272</td><td>2.654184</td><td>1.816703</td><td>2.768797</td><td>3.046651</td></tr> <tr><td>10 B</td><td>1.616519</td><td>1.841047</td><td>1.792406</td><td>4.218497</td><td>2.904151</td></tr> <tr><td>11 B</td><td>2.785440</td><td>1.820047</td><td>1.821853</td><td>4.196818</td><td>1.867188</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 C</td><td>1.584591</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Re</td><td>2.181112</td><td>3.270352</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.868205</td><td>2.835367</td><td>2.423164</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.823158</td><td>2.769489</td><td>3.290582</td><td>1.860468</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.582450</td><td>1.605204</td><td>3.496643</td><td>2.875580</td><td>1.776518</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.638447	0.000000				3 B	2.751430	2.830220	0.000000			4 B	3.540311	3.896820	3.464098	0.000000		5 B	2.881986	1.815108	2.702647	3.033995	0.000000	6 B	2.754619	2.811602	1.829719	1.722740	1.959926	7 C	3.386131	2.749772	1.637665	3.178848	1.628390	8 Re	2.124482	2.381084	3.465957	2.029992	2.306030	9 B	1.601272	2.654184	1.816703	2.768797	3.046651	10 B	1.616519	1.841047	1.792406	4.218497	2.904151	11 B	2.785440	1.820047	1.821853	4.196818	1.867188		6	7	8	9	10	6 B	0.000000					7 C	1.584591	0.000000				8 Re	2.181112	3.270352	0.000000			9 B	1.868205	2.835367	2.423164	0.000000		10 B	2.823158	2.769489	3.290582	1.860468	0.000000	11 B	2.582450	1.605204	3.496643	2.875580	1.776518
	1	2	3	4	5																																																																																																														
1 C	0.000000																																																																																																																		
2 B	1.638447	0.000000																																																																																																																	
3 B	2.751430	2.830220	0.000000																																																																																																																
4 B	3.540311	3.896820	3.464098	0.000000																																																																																																															
5 B	2.881986	1.815108	2.702647	3.033995	0.000000																																																																																																														
6 B	2.754619	2.811602	1.829719	1.722740	1.959926																																																																																																														
7 C	3.386131	2.749772	1.637665	3.178848	1.628390																																																																																																														
8 Re	2.124482	2.381084	3.465957	2.029992	2.306030																																																																																																														
9 B	1.601272	2.654184	1.816703	2.768797	3.046651																																																																																																														
10 B	1.616519	1.841047	1.792406	4.218497	2.904151																																																																																																														
11 B	2.785440	1.820047	1.821853	4.196818	1.867188																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 C	1.584591	0.000000																																																																																																																	
8 Re	2.181112	3.270352	0.000000																																																																																																																
9 B	1.868205	2.835367	2.423164	0.000000																																																																																																															
10 B	2.823158	2.769489	3.290582	1.860468	0.000000																																																																																																														
11 B	2.582450	1.605204	3.496643	2.875580	1.776518																																																																																																														
 <p>9. -553.02024337 +17.8 Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.745615</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.644465</td><td>3.540172</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.912316</td><td>3.669892</td><td>1.755880</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.762145</td><td>2.937685</td><td>2.918148</td><td>1.749910</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.852314</td><td>1.773317</td><td>2.982891</td><td>2.872940</td><td>2.835209</td></tr> <tr><td>7 B</td><td>1.761633</td><td>2.937552</td><td>2.918609</td><td>1.749082</td><td>1.754506</td></tr> <tr><td>8 B</td><td>1.851547</td><td>1.773957</td><td>2.984756</td><td>2.874764</td><td>1.810136</td></tr> <tr><td>9 C</td><td>2.811634</td><td>2.979237</td><td>1.671666</td><td>1.729578</td><td>2.712660</td></tr> <tr><td>10 C</td><td>2.811803</td><td>2.979981</td><td>1.671135</td><td>1.729964</td><td>1.744648</td></tr> <tr><td>11 Re</td><td>3.152192</td><td>2.079048</td><td>2.072178</td><td>3.170935</td><td>3.359186</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>1.811000</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.713004</td><td>2.835113</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.677018</td><td>1.745708</td><td>3.080105</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>3.078716</td><td>2.712099</td><td>1.679224</td><td>2.457305</td><td>0.000000</td></tr> <tr><td>11 Re</td><td>2.333274</td><td>3.363842</td><td>2.325726</td><td>2.313293</td><td>2.305032</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.745615	0.000000				3 B	3.644465	3.540172	0.000000			4 B	2.912316	3.669892	1.755880	0.000000		5 B	1.762145	2.937685	2.918148	1.749910	0.000000	6 B	1.852314	1.773317	2.982891	2.872940	2.835209	7 B	1.761633	2.937552	2.918609	1.749082	1.754506	8 B	1.851547	1.773957	2.984756	2.874764	1.810136	9 C	2.811634	2.979237	1.671666	1.729578	2.712660	10 C	2.811803	2.979981	1.671135	1.729964	1.744648	11 Re	3.152192	2.079048	2.072178	3.170935	3.359186		6	7	8	9	10	6 B	0.000000					7 B	1.811000	0.000000				8 B	2.713004	2.835113	0.000000			9 C	1.677018	1.745708	3.080105	0.000000		10 C	3.078716	2.712099	1.679224	2.457305	0.000000	11 Re	2.333274	3.363842	2.325726	2.313293	2.305032
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.745615	0.000000																																																																																																																	
3 B	3.644465	3.540172	0.000000																																																																																																																
4 B	2.912316	3.669892	1.755880	0.000000																																																																																																															
5 B	1.762145	2.937685	2.918148	1.749910	0.000000																																																																																																														
6 B	1.852314	1.773317	2.982891	2.872940	2.835209																																																																																																														
7 B	1.761633	2.937552	2.918609	1.749082	1.754506																																																																																																														
8 B	1.851547	1.773957	2.984756	2.874764	1.810136																																																																																																														
9 C	2.811634	2.979237	1.671666	1.729578	2.712660																																																																																																														
10 C	2.811803	2.979981	1.671135	1.729964	1.744648																																																																																																														
11 Re	3.152192	2.079048	2.072178	3.170935	3.359186																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.811000	0.000000																																																																																																																	
8 B	2.713004	2.835113	0.000000																																																																																																																
9 C	1.677018	1.745708	3.080105	0.000000																																																																																																															
10 C	3.078716	2.712099	1.679224	2.457305	0.000000																																																																																																														
11 Re	2.333274	3.363842	2.325726	2.313293	2.305032																																																																																																														

 <p>10. -553.01491520 +21.18 Cs</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>3.070843</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>3.445683</td><td>1.659457</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.764853</td><td>3.246632</td><td>2.913612</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.765122</td><td>2.933658</td><td>3.513570</td><td>1.842552</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.931363</td><td>1.815566</td><td>2.766019</td><td>2.840829</td><td>1.761373</td></tr> <tr><td>7 C</td><td>3.556455</td><td>1.779252</td><td>1.572774</td><td>2.797379</td><td>2.820839</td></tr> <tr><td>8 B</td><td>2.931363</td><td>2.862691</td><td>2.766019</td><td>1.795248</td><td>1.761373</td></tr> <tr><td>9 B</td><td>3.070843</td><td>2.749000</td><td>1.659457</td><td>1.750083</td><td>2.933658</td></tr> <tr><td>10 Re</td><td>2.093840</td><td>2.349871</td><td>2.019302</td><td>2.354183</td><td>3.164361</td></tr> <tr><td>11 B</td><td>1.764803</td><td>1.750183</td><td>2.913699</td><td>2.720200</td><td>1.842516</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 C</td><td>1.694081</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.782000</td><td>1.694081</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.862691</td><td>1.779252</td><td>1.815566</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.329123</td><td>3.035192</td><td>3.329123</td><td>2.349871</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.795292</td><td>2.797456</td><td>2.840857</td><td>3.246686</td><td>2.354225</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.070843	0.000000				3 C	3.445683	1.659457	0.000000			4 B	1.764853	3.246632	2.913612	0.000000		5 B	1.765122	2.933658	3.513570	1.842552	0.000000	6 B	2.931363	1.815566	2.766019	2.840829	1.761373	7 C	3.556455	1.779252	1.572774	2.797379	2.820839	8 B	2.931363	2.862691	2.766019	1.795248	1.761373	9 B	3.070843	2.749000	1.659457	1.750083	2.933658	10 Re	2.093840	2.349871	2.019302	2.354183	3.164361	11 B	1.764803	1.750183	2.913699	2.720200	1.842516		6	7	8	9	10	6 B	0.000000					7 C	1.694081	0.000000				8 B	1.782000	1.694081	0.000000			9 B	2.862691	1.779252	1.815566	0.000000		10 Re	3.329123	3.035192	3.329123	2.349871	0.000000	11 B	1.795292	2.797456	2.840857	3.246686	2.354225
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	3.070843	0.000000																																																																																																																	
3 C	3.445683	1.659457	0.000000																																																																																																																
4 B	1.764853	3.246632	2.913612	0.000000																																																																																																															
5 B	1.765122	2.933658	3.513570	1.842552	0.000000																																																																																																														
6 B	2.931363	1.815566	2.766019	2.840829	1.761373																																																																																																														
7 C	3.556455	1.779252	1.572774	2.797379	2.820839																																																																																																														
8 B	2.931363	2.862691	2.766019	1.795248	1.761373																																																																																																														
9 B	3.070843	2.749000	1.659457	1.750083	2.933658																																																																																																														
10 Re	2.093840	2.349871	2.019302	2.354183	3.164361																																																																																																														
11 B	1.764803	1.750183	2.913699	2.720200	1.842516																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 C	1.694081	0.000000																																																																																																																	
8 B	1.782000	1.694081	0.000000																																																																																																																
9 B	2.862691	1.779252	1.815566	0.000000																																																																																																															
10 Re	3.329123	3.035192	3.329123	2.349871	0.000000																																																																																																														
11 B	1.795292	2.797456	2.840857	3.246686	2.354225																																																																																																														
 <p>11. -553.01411866 +21.7</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 C</td><td>2.983189</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>3.435523</td><td>1.567036</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.765662</td><td>3.090918</td><td>2.902381</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.764045</td><td>2.797954</td><td>3.493108</td><td>1.835246</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.951003</td><td>1.734159</td><td>2.756465</td><td>2.823277</td><td>1.752981</td></tr> <tr><td>7 B</td><td>3.723261</td><td>1.776455</td><td>1.649458</td><td>2.915535</td><td>2.945889</td></tr> <tr><td>8 B</td><td>2.949841</td><td>2.718499</td><td>2.770827</td><td>1.793474</td><td>1.775405</td></tr> <tr><td>9 B</td><td>3.086199</td><td>2.591835</td><td>1.641678</td><td>1.768205</td><td>2.943424</td></tr> <tr><td>10 Re</td><td>2.078329</td><td>2.311059</td><td>2.037647</td><td>2.353001</td><td>3.154785</td></tr> <tr><td>11 B</td><td>1.782680</td><td>1.671369</td><td>2.860223</td><td>2.709634</td><td>1.845510</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.775998</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.766323</td><td>1.766580</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.848391</td><td>1.838733</td><td>1.828986</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.356714</td><td>3.205856</td><td>3.354739</td><td>2.367063</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.816500</td><td>2.925506</td><td>2.848892</td><td>3.224241</td><td>2.331327</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	2.983189	0.000000				3 C	3.435523	1.567036	0.000000			4 B	1.765662	3.090918	2.902381	0.000000		5 B	1.764045	2.797954	3.493108	1.835246	0.000000	6 B	2.951003	1.734159	2.756465	2.823277	1.752981	7 B	3.723261	1.776455	1.649458	2.915535	2.945889	8 B	2.949841	2.718499	2.770827	1.793474	1.775405	9 B	3.086199	2.591835	1.641678	1.768205	2.943424	10 Re	2.078329	2.311059	2.037647	2.353001	3.154785	11 B	1.782680	1.671369	2.860223	2.709634	1.845510		6	7	8	9	10	6 B	0.000000					7 B	1.775998	0.000000				8 B	1.766323	1.766580	0.000000			9 B	2.848391	1.838733	1.828986	0.000000		10 Re	3.356714	3.205856	3.354739	2.367063	0.000000	11 B	1.816500	2.925506	2.848892	3.224241	2.331327
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 C	2.983189	0.000000																																																																																																																	
3 C	3.435523	1.567036	0.000000																																																																																																																
4 B	1.765662	3.090918	2.902381	0.000000																																																																																																															
5 B	1.764045	2.797954	3.493108	1.835246	0.000000																																																																																																														
6 B	2.951003	1.734159	2.756465	2.823277	1.752981																																																																																																														
7 B	3.723261	1.776455	1.649458	2.915535	2.945889																																																																																																														
8 B	2.949841	2.718499	2.770827	1.793474	1.775405																																																																																																														
9 B	3.086199	2.591835	1.641678	1.768205	2.943424																																																																																																														
10 Re	2.078329	2.311059	2.037647	2.353001	3.154785																																																																																																														
11 B	1.782680	1.671369	2.860223	2.709634	1.845510																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.775998	0.000000																																																																																																																	
8 B	1.766323	1.766580	0.000000																																																																																																																
9 B	2.848391	1.838733	1.828986	0.000000																																																																																																															
10 Re	3.356714	3.205856	3.354739	2.367063	0.000000																																																																																																														
11 B	1.816500	2.925506	2.848892	3.224241	2.331327																																																																																																														

 <p>12. -553.00229130 +29.1</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 C</td><td>1.655732</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.529521</td><td>2.948782</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.774523</td><td>3.081717</td><td>1.754996</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.752969</td><td>2.582927</td><td>3.052304</td><td>1.755045</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.703637</td><td>1.743757</td><td>2.928241</td><td>2.827692</td><td>2.859571</td></tr> <tr><td>7 B</td><td>1.686845</td><td>2.706645</td><td>2.924794</td><td>1.784978</td><td>1.818247</td></tr> <tr><td>8 B</td><td>1.691621</td><td>1.689877</td><td>3.577286</td><td>3.067460</td><td>1.758529</td></tr> <tr><td>9 B</td><td>2.810121</td><td>2.791066</td><td>1.760493</td><td>1.840922</td><td>2.937093</td></tr> <tr><td>10 Re</td><td>3.014411</td><td>2.267406</td><td>2.093494</td><td>2.365913</td><td>2.333448</td></tr> <tr><td>11 B</td><td>2.773091</td><td>1.662466</td><td>1.773151</td><td>2.719465</td><td>3.221692</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>1.772807</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.941666</td><td>2.932358</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.741532</td><td>1.772069</td><td>3.687032</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.347011</td><td>3.332432</td><td>2.077910</td><td>3.168401</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.813558</td><td>2.849055</td><td>3.024434</td><td>1.854491</td><td>2.335770</td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 C	1.655732	0.000000				3 B	3.529521	2.948782	0.000000			4 B	2.774523	3.081717	1.754996	0.000000		5 B	1.752969	2.582927	3.052304	1.755045	0.000000	6 B	1.703637	1.743757	2.928241	2.827692	2.859571	7 B	1.686845	2.706645	2.924794	1.784978	1.818247	8 B	1.691621	1.689877	3.577286	3.067460	1.758529	9 B	2.810121	2.791066	1.760493	1.840922	2.937093	10 Re	3.014411	2.267406	2.093494	2.365913	2.333448	11 B	2.773091	1.662466	1.773151	2.719465	3.221692		6	7	8	9	10	6 B	0.000000					7 B	1.772807	0.000000				8 B	2.941666	2.932358	0.000000			9 B	1.741532	1.772069	3.687032	0.000000		10 Re	3.347011	3.332432	2.077910	3.168401	0.000000	11 B	1.813558	2.849055	3.024434	1.854491	2.335770
	1	2	3	4	5																																																																																																														
1 C	0.000000																																																																																																																		
2 C	1.655732	0.000000																																																																																																																	
3 B	3.529521	2.948782	0.000000																																																																																																																
4 B	2.774523	3.081717	1.754996	0.000000																																																																																																															
5 B	1.752969	2.582927	3.052304	1.755045	0.000000																																																																																																														
6 B	1.703637	1.743757	2.928241	2.827692	2.859571																																																																																																														
7 B	1.686845	2.706645	2.924794	1.784978	1.818247																																																																																																														
8 B	1.691621	1.689877	3.577286	3.067460	1.758529																																																																																																														
9 B	2.810121	2.791066	1.760493	1.840922	2.937093																																																																																																														
10 Re	3.014411	2.267406	2.093494	2.365913	2.333448																																																																																																														
11 B	2.773091	1.662466	1.773151	2.719465	3.221692																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.772807	0.000000																																																																																																																	
8 B	2.941666	2.932358	0.000000																																																																																																																
9 B	1.741532	1.772069	3.687032	0.000000																																																																																																															
10 Re	3.347011	3.332432	2.077910	3.168401	0.000000																																																																																																														
11 B	1.813558	2.849055	3.024434	1.854491	2.335770																																																																																																														
 <p>13. -553.00187194 +29.4</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.827572</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.711043</td><td>1.831122</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>2.794119</td><td>2.817877</td><td>2.796941</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.223106</td><td>2.919590</td><td>1.753130</td><td>1.764777</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.748881</td><td>2.933019</td><td>3.242989</td><td>1.792778</td><td>2.724728</td></tr> <tr><td>7 B</td><td>1.748808</td><td>1.759699</td><td>1.764541</td><td>3.547007</td><td>3.052652</td></tr> <tr><td>8 B</td><td>3.073247</td><td>3.691441</td><td>3.088341</td><td>1.669661</td><td>1.758754</td></tr> <tr><td>9 Re</td><td>2.338795</td><td>3.152099</td><td>2.367798</td><td>2.997870</td><td>2.315767</td></tr> <tr><td>10 C</td><td>1.716695</td><td>1.687153</td><td>2.697449</td><td>1.616110</td><td>2.708847</td></tr> <tr><td>11 B</td><td>2.846085</td><td>1.771636</td><td>1.780283</td><td>1.700967</td><td>1.800106</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>3.047461</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.749217</td><td>3.609321</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Re</td><td>2.286443</td><td>2.099774</td><td>2.093059</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>1.761607</td><td>2.805977</td><td>2.798672</td><td>3.158002</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.883849</td><td>2.930725</td><td>2.919231</td><td>3.310148</td><td>1.711614</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.827572	0.000000				3 B	2.711043	1.831122	0.000000			4 C	2.794119	2.817877	2.796941	0.000000		5 B	3.223106	2.919590	1.753130	1.764777	0.000000	6 B	1.748881	2.933019	3.242989	1.792778	2.724728	7 B	1.748808	1.759699	1.764541	3.547007	3.052652	8 B	3.073247	3.691441	3.088341	1.669661	1.758754	9 Re	2.338795	3.152099	2.367798	2.997870	2.315767	10 C	1.716695	1.687153	2.697449	1.616110	2.708847	11 B	2.846085	1.771636	1.780283	1.700967	1.800106		6	7	8	9	10	6 B	0.000000					7 B	3.047461	0.000000				8 B	1.749217	3.609321	0.000000			9 Re	2.286443	2.099774	2.093059	0.000000		10 C	1.761607	2.805977	2.798672	3.158002	0.000000	11 B	2.883849	2.930725	2.919231	3.310148	1.711614
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.827572	0.000000																																																																																																																	
3 B	2.711043	1.831122	0.000000																																																																																																																
4 C	2.794119	2.817877	2.796941	0.000000																																																																																																															
5 B	3.223106	2.919590	1.753130	1.764777	0.000000																																																																																																														
6 B	1.748881	2.933019	3.242989	1.792778	2.724728																																																																																																														
7 B	1.748808	1.759699	1.764541	3.547007	3.052652																																																																																																														
8 B	3.073247	3.691441	3.088341	1.669661	1.758754																																																																																																														
9 Re	2.338795	3.152099	2.367798	2.997870	2.315767																																																																																																														
10 C	1.716695	1.687153	2.697449	1.616110	2.708847																																																																																																														
11 B	2.846085	1.771636	1.780283	1.700967	1.800106																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	3.047461	0.000000																																																																																																																	
8 B	1.749217	3.609321	0.000000																																																																																																																
9 Re	2.286443	2.099774	2.093059	0.000000																																																																																																															
10 C	1.761607	2.805977	2.798672	3.158002	0.000000																																																																																																														
11 B	2.883849	2.930725	2.919231	3.310148	1.711614																																																																																																														

 <p>14. -553.00127114 +29.7</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 C</td><td>1.584782</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.632468</td><td>1.608336</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.826517</td><td>2.769568</td><td>2.910586</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.945587</td><td>1.613704</td><td>1.873357</td><td>1.918732</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.816838</td><td>1.605466</td><td>1.866239</td><td>2.851009</td><td>2.671923</td></tr> <tr><td>7 B</td><td>2.884561</td><td>2.800426</td><td>1.846989</td><td>2.659700</td><td>2.927257</td></tr> <tr><td>8 B</td><td>3.623425</td><td>4.255537</td><td>3.744930</td><td>1.840957</td><td>3.108373</td></tr> <tr><td>9 C</td><td>2.854115</td><td>3.481081</td><td>2.935029</td><td>1.731480</td><td>3.008819</td></tr> <tr><td>10 Re</td><td>3.491033</td><td>3.311200</td><td>2.260489</td><td>2.373258</td><td>2.246936</td></tr> <tr><td>11 B</td><td>1.768531</td><td>2.726832</td><td>2.871084</td><td>1.872410</td><td>2.938163</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>1.857332</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>4.169521</td><td>3.094481</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>2.811318</td><td>1.644872</td><td>1.745551</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.477841</td><td>2.319752</td><td>1.978287</td><td>2.194168</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.758866</td><td>1.906548</td><td>3.064496</td><td>1.635294</td><td>3.273451</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.584782	0.000000				3 B	2.632468	1.608336	0.000000			4 B	1.826517	2.769568	2.910586	0.000000		5 B	1.945587	1.613704	1.873357	1.918732	0.000000	6 B	1.816838	1.605466	1.866239	2.851009	2.671923	7 B	2.884561	2.800426	1.846989	2.659700	2.927257	8 B	3.623425	4.255537	3.744930	1.840957	3.108373	9 C	2.854115	3.481081	2.935029	1.731480	3.008819	10 Re	3.491033	3.311200	2.260489	2.373258	2.246936	11 B	1.768531	2.726832	2.871084	1.872410	2.938163		6	7	8	9	10	6 B	0.000000					7 B	1.857332	0.000000				8 B	4.169521	3.094481	0.000000			9 C	2.811318	1.644872	1.745551	0.000000		10 Re	3.477841	2.319752	1.978287	2.194168	0.000000	11 B	1.758866	1.906548	3.064496	1.635294	3.273451
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 C	1.584782	0.000000																																																																																																																	
3 B	2.632468	1.608336	0.000000																																																																																																																
4 B	1.826517	2.769568	2.910586	0.000000																																																																																																															
5 B	1.945587	1.613704	1.873357	1.918732	0.000000																																																																																																														
6 B	1.816838	1.605466	1.866239	2.851009	2.671923																																																																																																														
7 B	2.884561	2.800426	1.846989	2.659700	2.927257																																																																																																														
8 B	3.623425	4.255537	3.744930	1.840957	3.108373																																																																																																														
9 C	2.854115	3.481081	2.935029	1.731480	3.008819																																																																																																														
10 Re	3.491033	3.311200	2.260489	2.373258	2.246936																																																																																																														
11 B	1.768531	2.726832	2.871084	1.872410	2.938163																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.857332	0.000000																																																																																																																	
8 B	4.169521	3.094481	0.000000																																																																																																																
9 C	2.811318	1.644872	1.745551	0.000000																																																																																																															
10 Re	3.477841	2.319752	1.978287	2.194168	0.000000																																																																																																														
11 B	1.758866	1.906548	3.064496	1.635294	3.273451																																																																																																														
 <p>15. -553.00046850 +30.3</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.758276</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.792503</td><td>2.702191</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.587473</td><td>3.099115</td><td>2.818664</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.060676</td><td>1.777508</td><td>2.683233</td><td>1.768641</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.015266</td><td>3.240171</td><td>1.767929</td><td>1.753697</td><td>2.712373</td></tr> <tr><td>7 B</td><td>3.669096</td><td>2.947607</td><td>1.674802</td><td>1.750353</td><td>1.842487</td></tr> <tr><td>8 Re</td><td>2.089624</td><td>2.360223</td><td>3.187190</td><td>2.088878</td><td>2.344223</td></tr> <tr><td>9 C</td><td>1.663681</td><td>2.580558</td><td>1.659093</td><td>2.956826</td><td>3.076124</td></tr> <tr><td>10 B</td><td>1.745637</td><td>1.823102</td><td>1.695760</td><td>3.702901</td><td>2.909856</td></tr> <tr><td>11 B</td><td>2.925636</td><td>1.806667</td><td>1.682084</td><td>2.933179</td><td>1.779549</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>1.847562</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Re</td><td>2.309348</td><td>3.141367</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.678721</td><td>2.785907</td><td>2.260069</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.931929</td><td>2.936095</td><td>3.160516</td><td>1.765000</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.865053</td><td>1.777766</td><td>3.320609</td><td>2.714842</td><td>1.770153</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.758276	0.000000				3 C	2.792503	2.702191	0.000000			4 B	3.587473	3.099115	2.818664	0.000000		5 B	3.060676	1.777508	2.683233	1.768641	0.000000	6 B	3.015266	3.240171	1.767929	1.753697	2.712373	7 B	3.669096	2.947607	1.674802	1.750353	1.842487	8 Re	2.089624	2.360223	3.187190	2.088878	2.344223	9 C	1.663681	2.580558	1.659093	2.956826	3.076124	10 B	1.745637	1.823102	1.695760	3.702901	2.909856	11 B	2.925636	1.806667	1.682084	2.933179	1.779549		6	7	8	9	10	6 B	0.000000					7 B	1.847562	0.000000				8 Re	2.309348	3.141367	0.000000			9 C	1.678721	2.785907	2.260069	0.000000		10 B	2.931929	2.936095	3.160516	1.765000	0.000000	11 B	2.865053	1.777766	3.320609	2.714842	1.770153
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.758276	0.000000																																																																																																																	
3 C	2.792503	2.702191	0.000000																																																																																																																
4 B	3.587473	3.099115	2.818664	0.000000																																																																																																															
5 B	3.060676	1.777508	2.683233	1.768641	0.000000																																																																																																														
6 B	3.015266	3.240171	1.767929	1.753697	2.712373																																																																																																														
7 B	3.669096	2.947607	1.674802	1.750353	1.842487																																																																																																														
8 Re	2.089624	2.360223	3.187190	2.088878	2.344223																																																																																																														
9 C	1.663681	2.580558	1.659093	2.956826	3.076124																																																																																																														
10 B	1.745637	1.823102	1.695760	3.702901	2.909856																																																																																																														
11 B	2.925636	1.806667	1.682084	2.933179	1.779549																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.847562	0.000000																																																																																																																	
8 Re	2.309348	3.141367	0.000000																																																																																																																
9 C	1.678721	2.785907	2.260069	0.000000																																																																																																															
10 B	2.931929	2.936095	3.160516	1.765000	0.000000																																																																																																														
11 B	2.865053	1.777766	3.320609	2.714842	1.770153																																																																																																														

 <p>16. -553.00037778 +30.3 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>1.875247</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.702633</td><td>1.823114</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.841574</td><td>1.926153</td><td>2.729604</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>1.561553</td><td>1.629089</td><td>1.580469</td><td>2.641922</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.007439</td><td>1.723529</td><td>1.838500</td><td>1.898101</td><td>2.759964</td></tr> <tr><td>7 B</td><td>3.580878</td><td>3.006925</td><td>1.849600</td><td>2.729604</td><td>3.087379</td></tr> <tr><td>8 B</td><td>2.983600</td><td>3.569321</td><td>3.580878</td><td>1.841574</td><td>3.712826</td></tr> <tr><td>9 C</td><td>3.712826</td><td>3.796120</td><td>3.087379</td><td>2.641922</td><td>3.803000</td></tr> <tr><td>10 Re</td><td>2.142769</td><td>3.020767</td><td>2.434725</td><td>2.403081</td><td>2.214379</td></tr> <tr><td>11 B</td><td>3.569321</td><td>3.091400</td><td>3.006925</td><td>1.926153</td><td>3.796120</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>1.838500</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.007439</td><td>2.702633</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>2.759964</td><td>1.580469</td><td>1.561553</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.109792</td><td>2.434725</td><td>2.142769</td><td>2.214379</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.723529</td><td>1.823114</td><td>1.875247</td><td>1.629089</td><td>3.020767</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.875247	0.000000				3 B	2.702633	1.823114	0.000000			4 B	1.841574	1.926153	2.729604	0.000000		5 C	1.561553	1.629089	1.580469	2.641922	0.000000	6 B	3.007439	1.723529	1.838500	1.898101	2.759964	7 B	3.580878	3.006925	1.849600	2.729604	3.087379	8 B	2.983600	3.569321	3.580878	1.841574	3.712826	9 C	3.712826	3.796120	3.087379	2.641922	3.803000	10 Re	2.142769	3.020767	2.434725	2.403081	2.214379	11 B	3.569321	3.091400	3.006925	1.926153	3.796120		6	7	8	9	10	6 B	0.000000					7 B	1.838500	0.000000				8 B	3.007439	2.702633	0.000000			9 C	2.759964	1.580469	1.561553	0.000000		10 Re	3.109792	2.434725	2.142769	2.214379	0.000000	11 B	1.723529	1.823114	1.875247	1.629089	3.020767
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.875247	0.000000																																																																																																																	
3 B	2.702633	1.823114	0.000000																																																																																																																
4 B	1.841574	1.926153	2.729604	0.000000																																																																																																															
5 C	1.561553	1.629089	1.580469	2.641922	0.000000																																																																																																														
6 B	3.007439	1.723529	1.838500	1.898101	2.759964																																																																																																														
7 B	3.580878	3.006925	1.849600	2.729604	3.087379																																																																																																														
8 B	2.983600	3.569321	3.580878	1.841574	3.712826																																																																																																														
9 C	3.712826	3.796120	3.087379	2.641922	3.803000																																																																																																														
10 Re	2.142769	3.020767	2.434725	2.403081	2.214379																																																																																																														
11 B	3.569321	3.091400	3.006925	1.926153	3.796120																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.838500	0.000000																																																																																																																	
8 B	3.007439	2.702633	0.000000																																																																																																																
9 C	2.759964	1.580469	1.561553	0.000000																																																																																																															
10 Re	3.109792	2.434725	2.142769	2.214379	0.000000																																																																																																														
11 B	1.723529	1.823114	1.875247	1.629089	3.020767																																																																																																														
 <p>17. -552.99977016 +30.7 (C_{2v}) 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>1.752167</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.080719</td><td>1.765200</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.752308</td><td>2.695204</td><td>3.221426</td><td>0.000000</td><td></td></tr> <tr><td>5 Re</td><td>2.103555</td><td>2.317284</td><td>2.317284</td><td>2.324975</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.740174</td><td>1.836793</td><td>2.934838</td><td>1.836778</td><td>3.137853</td></tr> <tr><td>7 C</td><td>2.812010</td><td>1.721636</td><td>1.721636</td><td>2.700395</td><td>3.147945</td></tr> <tr><td>8 B</td><td>3.079972</td><td>3.221426</td><td>2.695204</td><td>1.763800</td><td>2.324975</td></tr> <tr><td>9 B</td><td>3.718163</td><td>2.934838</td><td>1.836793</td><td>2.934121</td><td>3.137853</td></tr> <tr><td>10 B</td><td>3.637400</td><td>3.080719</td><td>1.752167</td><td>3.079972</td><td>2.103555</td></tr> <tr><td>11 C</td><td>2.811904</td><td>2.699600</td><td>2.699600</td><td>1.722346</td><td>3.151640</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 C</td><td>1.710780</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.934121</td><td>2.700395</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.968200</td><td>1.710780</td><td>1.836778</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.718163</td><td>2.812010</td><td>1.752308</td><td>1.740174</td><td>0.000000</td></tr> <tr><td>11 C</td><td>1.709932</td><td>1.604604</td><td>1.722346</td><td>1.709932</td><td>2.811904</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.752167	0.000000				3 B	3.080719	1.765200	0.000000			4 B	1.752308	2.695204	3.221426	0.000000		5 Re	2.103555	2.317284	2.317284	2.324975	0.000000	6 B	1.740174	1.836793	2.934838	1.836778	3.137853	7 C	2.812010	1.721636	1.721636	2.700395	3.147945	8 B	3.079972	3.221426	2.695204	1.763800	2.324975	9 B	3.718163	2.934838	1.836793	2.934121	3.137853	10 B	3.637400	3.080719	1.752167	3.079972	2.103555	11 C	2.811904	2.699600	2.699600	1.722346	3.151640		6	7	8	9	10	6 B	0.000000					7 C	1.710780	0.000000				8 B	2.934121	2.700395	0.000000			9 B	2.968200	1.710780	1.836778	0.000000		10 B	3.718163	2.812010	1.752308	1.740174	0.000000	11 C	1.709932	1.604604	1.722346	1.709932	2.811904
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 B	1.752167	0.000000																																																																																																																	
3 B	3.080719	1.765200	0.000000																																																																																																																
4 B	1.752308	2.695204	3.221426	0.000000																																																																																																															
5 Re	2.103555	2.317284	2.317284	2.324975	0.000000																																																																																																														
6 B	1.740174	1.836793	2.934838	1.836778	3.137853																																																																																																														
7 C	2.812010	1.721636	1.721636	2.700395	3.147945																																																																																																														
8 B	3.079972	3.221426	2.695204	1.763800	2.324975																																																																																																														
9 B	3.718163	2.934838	1.836793	2.934121	3.137853																																																																																																														
10 B	3.637400	3.080719	1.752167	3.079972	2.103555																																																																																																														
11 C	2.811904	2.699600	2.699600	1.722346	3.151640																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 C	1.710780	0.000000																																																																																																																	
8 B	2.934121	2.700395	0.000000																																																																																																																
9 B	2.968200	1.710780	1.836778	0.000000																																																																																																															
10 B	3.718163	2.812010	1.752308	1.740174	0.000000																																																																																																														
11 C	1.709932	1.604604	1.722346	1.709932	2.811904																																																																																																														

 <p>18. -552.99702402 +32.4 Cs</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 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.336687</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.336619</td><td>2.911000</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.443257</td><td>2.813401</td><td>2.813413</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.214648</td><td>1.835688</td><td>3.420544</td><td>1.986203</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.214648</td><td>3.420507</td><td>1.835756</td><td>1.986203</td><td>2.861600</td></tr> <tr><td>7 C</td><td>3.480313</td><td>2.780181</td><td>2.780247</td><td>1.731566</td><td>1.553171</td></tr> <tr><td>8 B</td><td>2.058273</td><td>1.756852</td><td>3.479684</td><td>1.894697</td><td>1.778618</td></tr> <tr><td>9 B</td><td>2.058273</td><td>3.479698</td><td>1.756824</td><td>1.894697</td><td>3.468740</td></tr> <tr><td>10 C</td><td>2.144626</td><td>1.593983</td><td>1.593977</td><td>3.057469</td><td>2.795066</td></tr> <tr><td>11 B</td><td>3.208920</td><td>2.061977</td><td>2.062048</td><td>2.719984</td><td>2.043023</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 C</td><td>1.553171</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.468740</td><td>2.800928</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.778618</td><td>2.800928</td><td>3.099200</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>2.795066</td><td>2.884695</td><td>2.822620</td><td>2.822620</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.043023</td><td>1.642287</td><td>3.062739</td><td>3.062739</td><td>1.648019</td></tr> </tbody> </table>		1	2	3	4	5	1 Re	0.000000					2 B	2.336687	0.000000				3 B	2.336619	2.911000	0.000000			4 B	2.443257	2.813401	2.813413	0.000000		5 B	3.214648	1.835688	3.420544	1.986203	0.000000	6 B	3.214648	3.420507	1.835756	1.986203	2.861600	7 C	3.480313	2.780181	2.780247	1.731566	1.553171	8 B	2.058273	1.756852	3.479684	1.894697	1.778618	9 B	2.058273	3.479698	1.756824	1.894697	3.468740	10 C	2.144626	1.593983	1.593977	3.057469	2.795066	11 B	3.208920	2.061977	2.062048	2.719984	2.043023		6	7	8	9	10	6 B	0.000000					7 C	1.553171	0.000000				8 B	3.468740	2.800928	0.000000			9 B	1.778618	2.800928	3.099200	0.000000		10 C	2.795066	2.884695	2.822620	2.822620	0.000000	11 B	2.043023	1.642287	3.062739	3.062739	1.648019
	1	2	3	4	5																																																																																																														
1 Re	0.000000																																																																																																																		
2 B	2.336687	0.000000																																																																																																																	
3 B	2.336619	2.911000	0.000000																																																																																																																
4 B	2.443257	2.813401	2.813413	0.000000																																																																																																															
5 B	3.214648	1.835688	3.420544	1.986203	0.000000																																																																																																														
6 B	3.214648	3.420507	1.835756	1.986203	2.861600																																																																																																														
7 C	3.480313	2.780181	2.780247	1.731566	1.553171																																																																																																														
8 B	2.058273	1.756852	3.479684	1.894697	1.778618																																																																																																														
9 B	2.058273	3.479698	1.756824	1.894697	3.468740																																																																																																														
10 C	2.144626	1.593983	1.593977	3.057469	2.795066																																																																																																														
11 B	3.208920	2.061977	2.062048	2.719984	2.043023																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 C	1.553171	0.000000																																																																																																																	
8 B	3.468740	2.800928	0.000000																																																																																																																
9 B	1.778618	2.800928	3.099200	0.000000																																																																																																															
10 C	2.795066	2.884695	2.822620	2.822620	0.000000																																																																																																														
11 B	2.043023	1.642287	3.062739	3.062739	1.648019																																																																																																														
 <p>19. -552.99619660 +32.9 Cs</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 C</td><td>1.685839</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.504128</td><td>3.041532</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.914831</td><td>3.397346</td><td>1.847225</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.834857</td><td>2.790116</td><td>3.029322</td><td>1.795247</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.825455</td><td>1.678036</td><td>2.594269</td><td>2.784116</td><td>2.860083</td></tr> <tr><td>7 B</td><td>1.763878</td><td>2.808196</td><td>2.828510</td><td>1.761255</td><td>1.822107</td></tr> <tr><td>8 B</td><td>1.759524</td><td>1.756948</td><td>3.337793</td><td>3.050932</td><td>1.761468</td></tr> <tr><td>9 C</td><td>2.805450</td><td>2.881974</td><td>1.580585</td><td>1.689967</td><td>2.788323</td></tr> <tr><td>10 Re</td><td>3.488233</td><td>3.194712</td><td>2.182668</td><td>2.297254</td><td>2.359807</td></tr> <tr><td>11 B</td><td>2.640836</td><td>1.508781</td><td>2.172039</td><td>2.945124</td><td>2.730487</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>1.806199</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.858232</td><td>2.908398</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>1.637602</td><td>1.658167</td><td>3.459830</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>3.674388</td><td>3.473161</td><td>2.346202</td><td>3.218224</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.453636</td><td>3.211821</td><td>1.784383</td><td>2.821488</td><td>1.958024</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	1.685839	0.000000				3 B	3.504128	3.041532	0.000000			4 B	2.914831	3.397346	1.847225	0.000000		5 B	1.834857	2.790116	3.029322	1.795247	0.000000	6 B	1.825455	1.678036	2.594269	2.784116	2.860083	7 B	1.763878	2.808196	2.828510	1.761255	1.822107	8 B	1.759524	1.756948	3.337793	3.050932	1.761468	9 C	2.805450	2.881974	1.580585	1.689967	2.788323	10 Re	3.488233	3.194712	2.182668	2.297254	2.359807	11 B	2.640836	1.508781	2.172039	2.945124	2.730487		6	7	8	9	10	6 B	0.000000					7 B	1.806199	0.000000				8 B	2.858232	2.908398	0.000000			9 C	1.637602	1.658167	3.459830	0.000000		10 Re	3.674388	3.473161	2.346202	3.218224	0.000000	11 B	2.453636	3.211821	1.784383	2.821488	1.958024
	1	2	3	4	5																																																																																																														
1 B	0.000000																																																																																																																		
2 C	1.685839	0.000000																																																																																																																	
3 B	3.504128	3.041532	0.000000																																																																																																																
4 B	2.914831	3.397346	1.847225	0.000000																																																																																																															
5 B	1.834857	2.790116	3.029322	1.795247	0.000000																																																																																																														
6 B	1.825455	1.678036	2.594269	2.784116	2.860083																																																																																																														
7 B	1.763878	2.808196	2.828510	1.761255	1.822107																																																																																																														
8 B	1.759524	1.756948	3.337793	3.050932	1.761468																																																																																																														
9 C	2.805450	2.881974	1.580585	1.689967	2.788323																																																																																																														
10 Re	3.488233	3.194712	2.182668	2.297254	2.359807																																																																																																														
11 B	2.640836	1.508781	2.172039	2.945124	2.730487																																																																																																														
	6	7	8	9	10																																																																																																														
6 B	0.000000																																																																																																																		
7 B	1.806199	0.000000																																																																																																																	
8 B	2.858232	2.908398	0.000000																																																																																																																
9 C	1.637602	1.658167	3.459830	0.000000																																																																																																															
10 Re	3.674388	3.473161	2.346202	3.218224	0.000000																																																																																																														
11 B	2.453636	3.211821	1.784383	2.821488	1.958024																																																																																																														

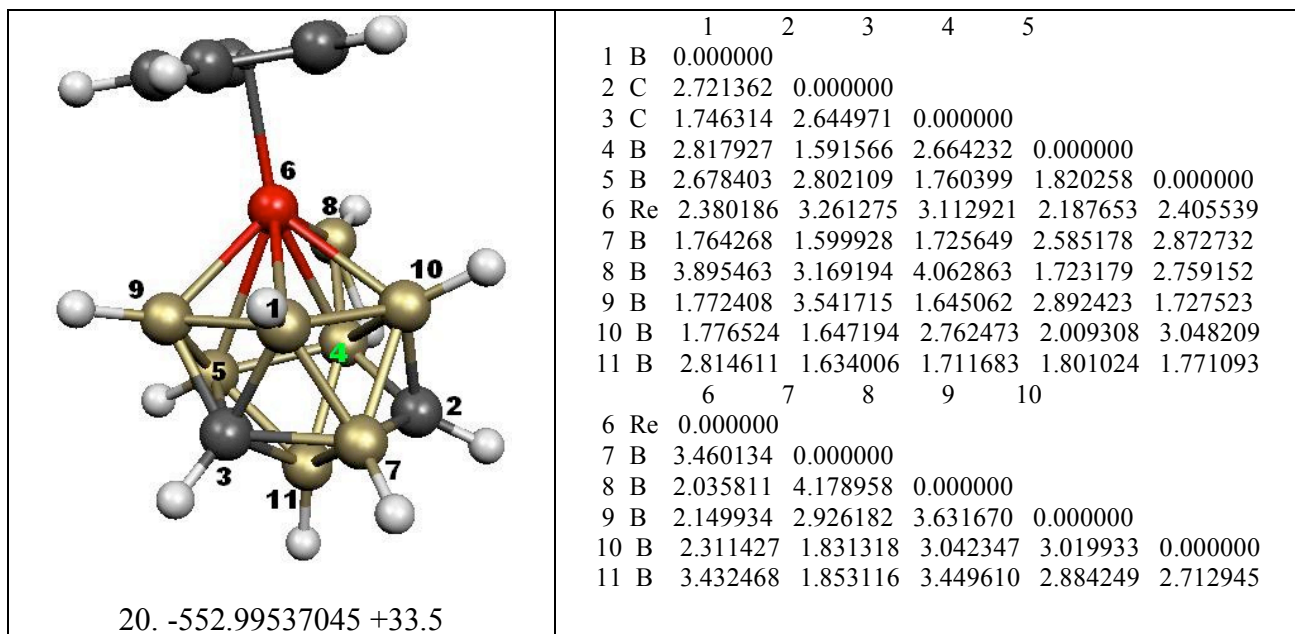


Table 4. Energy ranking

No	Initial structure	Final energy (a.u.)	D kcal/mole	Remarks
1	1-PentaCapTrPr_Re_v3_C2_v64b	-553.04867037	0.00	
2	1-PentaCapTrPr_Re_v4_C2_v66b	-553.04867037	0.00	
3	2-TricapCubeA_Re_v4a_C2_v55b	-553.04867037	0.00	
4	2-TricapCubeA_Re_v4b_C2_j	-553.04867037	0.00	
5	2-TricapCubeB_Re_v4_C2_u	-553.04867037	0.00	
6	4-Icos-1vx_Re_v4_C2_d	-553.04867037	0.00	
7	4-Icos-1vx_Re_v5a_C2_h	-553.04867037	0.00	
8	4-Icos-1vx_Re_v5b_C2_v	-553.04867037	0.00	
9	4-Icos-1vx_Re_v6_C2_f_r-9	-553.04867037	0.00	
10	4-Icos-1vx_Re_v6_C2_f	-553.04859667	0.05	
11	2-TricapCubeA_Re_v4a_C2_v54c	-553.04465894	2.52	
12	2-TricapCubeA_Re_v4b_C2_m	-553.04465894	2.52	
13	3-OhfusetopentBipyr_Re_v5_C2_u	-553.04465894	2.52	
14	4-Icos-1vx_Re_v4_C2_f	-553.04465894	2.52	
15	4-Icos-1vx_Re_v5a_C2_f	-553.04465894	2.52	
16	1-PentaCapTrPr_Re_v4_C2_v64b	-553.04465727	2.52	
17	1-PentaCapTrPr_Re_v6_C2_a	-553.04465727	2.52	
18	2-TricapCubeB_Re_v4_C2_c	-553.04465727	2.52	
19	4-Icos-1vx_Re_v5b_C2_l	-553.04465727	2.52	
20	4-Icos-1vx_Re_v4_C2_y	-553.04465726	2.52	
21	1-PentaCapTrPr_Re_v4_C2_v63d	-553.04463527	2.53	
22	4-Icos-1vx_Re_v6_C2_e	-553.04463527	2.53	
23	3-OhfusetopentBipyr_Re_v6b_C2_q	-553.04463520	2.53	
24	4-Icos-1vx_Re_v5a_C2_w	-553.04462961	2.54	
25	2-TricapCubeB_Re_v6_C2_j	-553.04462960	2.54	
26	4-Icos-1vx_Re_v4_C2_o	-553.03906771	6.03	
27	1-PentaCapTrPr_Re_v3_C2_v43	-553.03906770	6.03	
28	1-PentaCapTrPr_Re_v3_C2_v63a	-553.03906770	6.03	
29	1-PentaCapTrPr_Re_v4_C2_v66d	-553.03906770	6.03	
30	1-PentaCapTrPr_Re_v4_C2_v66e	-553.03906770	6.03	
31	2-TricapCubeA_Re_v4a_C2_v54b	-553.03906770	6.03	
32	2-TricapCubeA_Re_v4a_C2_v54d	-553.03906770	6.03	
33	2-TricapCubeB_Re_v4_C2_h	-553.03906770	6.03	
34	2-TricapCubeB_Re_v4_C2_m	-553.03906770	6.03	
35	2-TricapCubeB_Re_v6_C2_l	-553.03906770	6.03	
36	2-TricapCubeB_Re_v6_C2_r	-553.03906770	6.03	
37	4-Icos-1vx_Re_v4_C2_u	-553.03906770	6.03	
38	4-Icos-1vx_Re_v5a_C2_c	-553.03906770	6.03	

39	4-Icos-1vx_Re_v5a_C2_e	-553.03906770	6.03
40	4-Icos-1vx_Re_v5a_C2_zc	-553.03906770	6.03
41	4-Icos-1vx_Re_v5a_C2_zl	-553.03906770	6.03
42	4-Icos-1vx_Re_v5b_C2_o	-553.03906770	6.03
43	4-Icos-1vx_Re_v6_C2_c	-553.03906770	6.03
44	1-PentaCapTrPr_Re_v6_C2_d	-553.03906769	6.03
45	1-PentaCapTrPr_Re_v6_C2_j	-553.03906769	6.03
46	2-TricapCubeA_Re_v4a_C2_v54f	-553.03654077	7.61
47	4-Icos-1vx_Re_v5a_C2_p	-553.03654077	7.61
48	1-PentaCapTrPr_Re_v3_C2_v44	-553.03654076	7.61
49	1-PentaCapTrPr_Re_v6_C2_c	-553.03654076	7.61
50	3-OhfusetopentBipyr_Re_v6a_C2_zz	-553.03654076	7.61
51	4-Icos-1vx_Re_v4_C2_i	-553.03654076	7.61
52	4-Icos-1vx_Re_v5a_C2_zs	-553.03654076	7.61
53	4-Icos-1vx_Re_v5b_C2_f	-553.03654076	7.61
54	1-PentaCapTrPr_Re_v6_C2_o	-553.03654075	7.61
55	2-TricapCubeA_Re_v4b_C2_l	-553.03654075	7.61
56	2-TricapCubeB_Re_v4_C2_a	-553.03654075	7.61
57	4-Icos-1vx_Re_v5a_C2_d	-553.03654075	7.61
58	4-Icos-1vx_Re_v5b_C2_r	-553.03654075	7.61
59	4-Icos-1vx_Re_v6_C2_d	-553.03654075	7.61
60	4-Icos-1vx_Re_v5a_C2_g	-553.03654074	7.61
61	4-Icos-1vx_Re_v5a_C2_x	-553.03654074	7.61
62	4-Icos-1vx_Re_v5b_C2_u	-553.03654074	7.61
63	2-TricapCubeA_Re_v4a_C2_v55a	-553.03654070	7.61
64	1-PentaCapTrPr_Re_v4_C2_v44	-553.02844903	12.69
65	1-PentaCapTrPr_Re_v4_C2_v66f	-553.02844903	12.69
66	2-TricapCubeA_Re_v4a_C2_v54h	-553.02844903	12.69
67	2-TricapCubeB_Re_v4_C2_k	-553.02844903	12.69
68	4-Icos-1vx_Re_v6_C2_i	-553.02844903	12.69
69	1-PentaCapTrPr_Re_v6_C2_f	-553.02841866	12.71
70	1-PentaCapTrPr_Re_v6_C2_l	-553.02671402	13.78
71	1-PentaCapTrPr_Re_v6_C2_p	-553.02671402	13.78
72	2-TricapCubeB_Re_v4_C2_f	-553.02671402	13.78
73	2-TricapCubeB_Re_v4_C2_r	-553.02671402	13.78
74	3-OhfusetopentBipyr_Re_v6b_C2_v	-553.02671402	13.78
75	4-Icos-1vx_Re_v5a_C2_zp	-553.02671402	13.78
76	4-Icos-1vx_Re_v5b_C2_h	-553.02671402	13.78
77	4-Icos-1vx_Re_v5c_C2_k	-553.02671402	13.78
78	4-Icos-1vx_Re_v4_C2_l	-553.02262146	16.35
79	4-Icos-1vx_Re_v5a_C2_m	-553.02262146	16.35

80	4-Icos-1vx_Re_v5a_C2_zb	-553.02262146	16.35	
81	4-Icos-1vx_Re_v5a_C2_zd	-553.02262146	16.35	
82	4-Icos-1vx_Re_v5c_C2_zz	-553.02262146	16.35	
83	4-Icos-1vx_Re_v6_C2_l	-553.02262146	16.35	
84	2-TricapCubeB_Re_v4_C2_g	-553.02085934	17.45	
85	2-TricapCubeB_Re_v6_C2_b	-553.02085934	17.45	
86	1-PentaCapTrPr_Re_v6_C2_t	-553.02085933	17.45	
87	2-TricapCubeB_Re_v6_C2_v	-553.02085933	17.45	
88	4-Icos-1vx_Re_v6_C2_n	-553.02024337	17.84	
89	4-Icos-1vx_Re_v5a_C2_q	-553.02023657	17.84	
90	4-Icos-1vx_Re_v4_C2_q	-553.02023656	17.84	
91	2-TricapCubeA_Re_v4a_C2_v54a	-553.01491520	21.18	C-C
92	1-PentaCapTrPr_Re_v3_C2_v64c	-553.01491519	21.18	C-C
93	1-PentaCapTrPr_Re_v4_C2_v63c	-553.01491519	21.18	C-C
94	1-PentaCapTrPr_Re_v4_C2_v64a	-553.01491519	21.18	C-C
95	1-PentaCapTrPr_Re_v6_C2_b	-553.01491519	21.18	C-C
96	2-TricapCubeB_Re_v4_C2_b	-553.01491519	21.18	C-C
97	2-TricapCubeB_Re_v6_C2_o	-553.01491519	21.18	C-C
98	3-OhfusettoPentBipyr_Re_v6a_C2_l	-553.01491519	21.18	C-C
99	4-Icos-1vx_Re_v5a_C2_b	-553.01491519	21.18	C-C
100	4-Icos-1vx_Re_v5a_C2_zo	-553.01491519	21.18	C-C
101	4-Icos-1vx_Re_v5b_C2_s	-553.01491519	21.18	C-C
102	4-Icos-1vx_Re_v6_C2_a	-553.01491519	21.18	C-C
103	2-TricapCubeB_Re_v4_C2_j	-553.01411867	21.68	C-C
104	1-PentaCapTrPr_Re_v3_C2_v64a	-553.01411866	21.68	C-C
105	1-PentaCapTrPr_Re_v4_C2_v63a	-553.01411866	21.68	C-C
106	1-PentaCapTrPr_Re_v6_C2_e	-553.01411866	21.68	C-C
107	2-TricapCubeA_Re_v4a_C2_v54e	-553.01411866	21.68	C-C
108	2-TricapCubeA_Re_v4a_C2_v55c	-553.01411866	21.68	C-C
109	2-TricapCubeB_Re_v6_C2_n	-553.01411866	21.68	C-C
110	4-Icos-1vx_Re_v5a_C2_i	-553.01411866	21.68	C-C
111	4-Icos-1vx_Re_v5a_C2_zh	-553.01411866	21.68	C-C
112	4-Icos-1vx_Re_v5a_C2_zq	-553.01411866	21.68	C-C
113	2-TricapCubeB_Re_v4_C2_s	-553.01411865	21.68	C-C
114	2-TricapCubeB_Re_v4_C2_t	-553.01411865	21.68	C-C
115	4-Icos-1vx_Re_v5a_C2_a	-553.01411865	21.68	C-C
116	4-Icos-1vx_Re_v5b_C2_w	-553.01411865	21.68	C-C
117	4-Icos-1vx_Re_v6_C2_b	-553.01411865	21.68	C-C
118	4-Icos-1vx_Re_v5a_C2_zn	-553.00229130	29.10	C-C
119	4-Icos-1vx_Re_v4_C2_w	-553.00229129	29.10	C-C
120	4-Icos-1vx_Re_v5a_C2_j	-553.00229129	29.10	C-C

121	4-Icos-1vx_Re_v6_C2_g	-553.00229129	29.10	C-C
122	2-TricapCubeA_Re_v4a_C2_v54j	-553.00229128	29.10	C-C
123	3-OhfusetopentBipyr_Re_v6a_C2_o	-553.00229128	29.10	C-C
124	1-PentaCapTrPr_Re_v4_C2_v64c	-553.00187194	29.37	C-C
125	2-TricapCubeA_Re_v4a_C2_v54g	-553.00187194	29.37	C-C
126	2-TricapCubeA_Re_v4a_C2_v54i	-553.00187194	29.37	C-C
127	4-Icos-1vx_Re_v5a_C2_za	-553.00187194	29.37	C-C
128	4-Icos-1vx_Re_v6_C2_h	-553.00187194	29.37	C-C
129	2-TricapCubeB_Re_v6_C2_h	-553.00187193	29.37	C-C
130	3-OhfusetopentBipyr_Re_v6a_C2_r	-553.00127114	29.74	
131	2-TricapCubeB_Re_v4_C2_q	-553.00046850	30.25	C-C
132	4-Icos-1vx_Re_v5a_C2_zk	-553.00046850	30.25	C-C
133	4-Icos-1vx_Re_v6_C2_k	-553.00046850	30.25	C-C
134	4-Icos-1vx_Re_v4_C2_n	-553.00046849	30.25	C-C
135	4-Icos-1vx_Re_v5a_C2_k	-553.00046849	30.25	C-C
136	4-Icos-1vx_Re_v5a_C2_zm	-553.00046849	30.25	C-C
137	4-Icos-1vx_Re_v5c_C2_n	-553.00046849	30.25	C-C
138	3-OhfusetopentBipyr_Re_v6a_C2_c	-553.00037778	30.30	
139	3-OhfusetopentBipyr_Re_v6a_C2_f	-553.00037778	30.30	
140	1-PentaCapTrPr_Re_v4_C2_v33	-553.00037777	30.30	
141	3-OhfusetopentBipyr_Re_v5_C2_k	-553.00037777	30.30	
142	3-OhfusetopentBipyr_Re_v5_C2_o	-552.99977016	30.68	C-C
143	4-Icos-1vx_Re_v6_C2_j_r-12	-552.99977016	30.68	C-C
144	4-Icos-1vx_Re_v6_C2_j_i-12	-552.99972880	30.71	C-C
145	2-TricapCubeB_Re_v6_C2_w	-552.99773257	31.96	
146	2-TricapCubeB_Re_v6_C2_c	-552.99702402	32.41	
147	3-OhfusetopentBipyr_Re_v6a_C2_j	-552.99702402	32.41	
148	4-Icos-1vx_Re_v5a_C2_v	-552.99619660	32.93	
149	3-OhfusetopentBipyr_Re_v6a_C2_x	-552.99537046	33.45	
150	1-PentaCapTrPr_Re_v6_C2_s	-552.99537045	33.45	
151	1-PentaCapTrPr_Re_v6_C2_n	-552.99392740	34.35	
152	2-TricapCubeA_Re_v4b_C2_d	-552.99392740	34.35	C-C
153	4-Icos-1vx_Re_v5a_C2_l	-552.99392740	34.35	
154	4-Icos-1vx_Re_v5a_C2_zr	-552.99392740	34.35	C-C
155	4-Icos-1vx_Re_v5b_C2_g	-552.99392740	34.35	C-C
156	4-Icos-1vx_Re_v6_C2_m	-552.99392740	34.35	C-C
157	1-PentaCapTrPr_Re_v6_C2_h	-552.99380193	34.43	C-C
158	1-PentaCapTrPr_Re_v3_C2_v66d	-552.99332561	34.73	
159	2-TricapCubeB_Re_v6_C2_k	-552.99332561	34.73	
160	2-TricapCubeB_Re_v6_C2_zz	-552.99332561	34.73	
161	3-OhfusetopentBipyr_Re_v6a_C2_m	-552.99332561	34.73	

162	3-OhfusetopentBipyr_Re_v5_C2_p	-552.99332560	34.73	
163	4-Icos-1vx_Re_v4_C2_k	-552.99332560	34.73	
164	1-PentaCapTrPr_Re_v4_C2_v43	-552.99100662	36.18	
165	3-OhfusetopentBipyr_Re_v6b_C2_b	-552.99100658	36.18	
166	2-TricapCubeB_Re_v6_C2_q	-552.98948080	37.14	
167	2-TricapCubeB_Re_v6_C2_m	-552.98861877	37.68	
168	4-Icos-1vx_Re_v5c_C2_a	-552.98828669	37.89	
169	4-Icos-1vx_Re_v5c_C2_o	-552.98828669	37.89	
170	4-Icos-1vx_Re_v4_C2_zz	-552.98671907	38.87	
171	1-PentaCapTrPr_Re_v3_C2_v66c	-552.98589275	39.39	
172	2-TricapCubeB_Re_v6_C2_f	-552.98589275	39.39	
173	2-TricapCubeB_Re_v6_C2_y	-552.98589275	39.39	
174	3-OhfusetopentBipyr_Re_v6a_C2_n	-552.98589275	39.39	
175	2-TricapCubeB_Re_v4_C2_e	-552.98589274	39.39	
176	2-TricapCubeB_Re_v6_C2_e	-552.98544262	39.68	
177	2-TricapCubeB_Re_v6_C2_z	-552.98544262	39.68	
178	2-TricapCubeB_Re_v4_C2_v	-552.98446088	40.29	
179	3-OhfusetopentBipyr_Re_v5_C2_f	-552.98446088	40.29	
180	3-OhfusetopentBipyr_Re_v6a_C2_ur-27	-552.98446088	40.29	
181	1-PentaCapTrPr_Re_v6_C2_u	-552.98421413	40.45	
182	3-OhfusetopentBipyr_Re_v6a_C2_u i-27	-552.98395843	40.61	
183	4-Icos-1vx_Re_v5c_C2_f	-552.98091936	42.51	
184	4-Icos-1vx_Re_v5c_C2_r	-552.98091935	42.51	
185	3-OhfusetopentBipyr_Re_v4_C2_u	-552.97960274	43.34	
186	3-OhfusetopentBipyr_Re_v4_C2_j	-552.97960265	43.34	
187	1-PentaCapTrPr_Re_v4_C2_v63b	-552.97940459	43.46	
188	3-OhfusetopentBipyr_Re_v5_C2_j	-552.97812380	44.27	
189	3-OhfusetopentBipyr_Re_v5_C2_v	-552.97812379	44.27	
190	3-OhfusetopentBipyr_Re_v6a_C2_e	-552.97812379	44.27	
191	1-PentaCapTrPr_Re_v6_C2_r	-552.97800920	44.34	C-C
192	2-TricapCubeA_Re_v4b_C2_h	-552.97684815	45.07	
193	4-Icos-1vx_Re_v5b_C2_e	-552.97684815	45.07	
194	3-OhfusetopentBipyr_Re_v6b_C2_za	-552.97619443	45.48	
195	1-PentaCapTrPr_Re_v3_C2_v66a	-552.97619442	45.48	
196	2-TricapCubeB_Re_v4_C2_i	-552.97619442	45.48	
197	2-TricapCubeB_Re_v6_C2_d	-552.97551426	45.91	
198	2-TricapCubeB_Re_v6_C2_s	-552.97551426	45.91	
199	2-TricapCubeB_Re_v6_C2_u	-552.97386318	46.94	
200	1-PentaCapTrPr_Re_v3_C2_v64d	-552.97386317	46.94	
201	2-TricapCubeB_Re_v6_C2_g	-552.97386317	46.94	
202	3-OhfusetopentBipyr_Re_v6a_C2_b	-552.97386317	46.94	

203	4-Icos-1vx_Re_v4_C2_h	-552.97386317	46.94	
204	2-TricapCubeB_Re_v4_C2_y	-552.97331620	47.28	
205	2-TricapCubeA_Re_v4b_C2_x_r-16	-552.97297312	47.50	
206	2-TricapCubeA_Re_v4a_C2_v54k	-552.97297311	47.50	
207	2-TricapCubeA_Re_v4b_C2_x_i-16	-552.97295489	47.51	
208	4-Icos-1vx_Re_v4_C2_t	-552.97291500	47.54	
209	4-Icos-1vx_Re_v5b_C2_q	-552.97153561	48.40	
210	2-TricapCubeB_Re_v4_C2_z	-552.97002867	49.35	
211	3-OhfusettoPentBipyr_Re_v5_C2_b	-552.96997861	49.38	
212	4-Icos-1vx_Re_v5a_C2_u	-552.96983880	49.47	
213	4-Icos-1vx_Re_v4_C2_b	-552.96906947	49.95	
214	4-Icos-1vx_Re_v5c_C2_y	-552.96857248	50.26	
215	4-Icos-1vx_Re_v5a_C2_zg	-552.96857247	50.26	
216	4-Icos-1vx_Re_v4_C2_z	-552.96784065	50.72	C-C
217	4-Icos-1vx_Re_v5b_C2_t	-552.96784064	50.72	C-C
218	4-Icos-1vx_Re_v5c_C2_x	-552.96784064	50.72	C-C
219	1-PentaCapTrPr_Re_v6_C2_k	-552.96779766	50.75	C-C
220	4-Icos-1vx_Re_v4_C2_c	-552.96776089	50.77	
221	2-TricapCubeA_Re_v4b_C2_q	-552.96653046	51.54	
222	3-OhfusettoPentBipyr_Re_v6a_C2_v	-552.96599849	51.88	
223	2-TricapCubeB_Re_v4_C2_d	-552.96574090	52.04	C-C
224	1-PentaCapTrPr_Re_v6_C2_m	-552.96546119	52.21	
225	3-OhfusettoPentBipyr_Re_v6a_C2hr-109	-552.96546118	52.21	
226	2-TricapCubeA_Re_v4b_C2_i	-552.96359714	53.38	
227	4-Icos-1vx_Re_v5b_C2_a	-552.96359714	53.38	
228	4-Icos-1vx_Re_v5c_C2_m	-552.96359713	53.38	
229	4-Icos-1vx_Re_v5a_C2_o	-552.96358247	53.39	
230	1-PentaCapTrPr_Re_v4_C2_v66c	-552.96347309	53.46	
231	3-OhfusettoPentBipyr_Re_v6a_C2_t	-552.96338091	53.52	
232	2-TricapCubeA_Re_v4b_C2_o	-552.96239987	54.13	C-C
233	3-OhfusettoPentBipyr_Re_v4_C2_r	-552.96229616	54.20	C-C
234	2-TricapCubeA_Re_v4b_C2_a	-552.96195638	54.41	
235	4-Icos-1vx_Re_v5c_C2_h	-552.96189831	54.45	
236	3-OhfusettoPentBipyr_Re_v5_C2_g	-552.96105693	54.98	
237	2-TricapCubeA_Re_v4b_C2_w	-552.96039698	55.39	
238	2-TricapCubeB_Re_v4_C2_zz	-552.96039698	55.39	
239	4-Icos-1vx_Re_v4_C2_x	-552.96039698	55.39	
240	3-OhfusettoPentBipyr_Re_v6b_C2_j	-552.96014659	55.55	
241	1-PentaCapTrPr_Re_v4_C2_v66a	-552.96007908	55.59	
242	3-OhfusettoPentBipyr_Re_v5_C2_zz	-552.96007908	55.59	
243	4-Icos-1vx_Re_v5b_C2_p	-552.96007908	55.59	

244	3-OhfusetopentBipyr_Re_v5_C2_t	-552.95874207	56.43	
245	3-OhfusetopentBipyr_Re_v6a_C2_q	-552.95874207	56.43	
246	3-OhfusetopentBipyr_Re_v6b_C2_zb	-552.95874206	56.43	
247	4-Icos-1vx_Re_v5c_C2_q	-552.95804985	56.86	C-C
248	2-TricapCubeB_Re_v6_C2_x	-552.95756323	57.17	C-C
249	1-PentaCapTrPr_Re_v3_C2_v66b	-552.95756322	57.17	C-C
250	4-Icos-1vx_Re_v4_C2_a	-552.95756322	57.17	C-C
251	1-PentaCapTrPr_Re_v6_C2_q	-552.95706566	57.48	
252	3-OhfusetopentBipyr_Re_v6a_C2_y	-552.95627160	57.98	
253	4-Icos-1vx_Re_v5a_C2_ze	-552.95544389	58.50	
254	3-OhfusetopentBipyr_Re_v4_C2_d	-552.95493169	58.82	
255	2-TricapCubeA_Re_v4b_C2_t	-552.95480136	58.90	
256	4-Icos-1vx_Re_v5a_C2_s	-552.95480136	58.90	
257	4-Icos-1vx_Re_v5c_C2_d	-552.95470279	58.96	
258	3-OhfusetopentBipyr_Re_v4_C2_c	-552.95450492	59.09	
259	4-Icos-1vx_Re_v5a_C2_r	-552.95430732	59.21	C-C
260	4-Icos-1vx_Re_v5b_C2_n	-552.95430732	59.21	C-C
261	4-Icos-1vx_Re_v4_C2_s	-552.95430731	59.21	C-C
262	3-OhfusetopentBipyr_Re_v5_C2_s	-552.95392263	59.45	C-C
263	3-OhfusetopentBipyr_Re_v6a_C2_p	-552.95392263	59.45	C-C
264	3-OhfusetopentBipyr_Re_v5_C2_m	-552.95235564	60.44	
265	3-OhfusetopentBipyr_Re_v5_C2_i	-552.95207751	60.61	C-C
266	3-OhfusetopentBipyr_Re_v6b_C2_f	-552.95152834	60.96	
267	3-OhfusetopentBipyr_Re_v6a_C2_g	-552.95114852	61.19	C-C
268	3-OhfusetopentBipyr_Re_v4_C2_i	-552.95100253	61.29	
269	4-Icos-1vx_Re_v5b_C2_k	-552.95100252	61.29	
270	3-OhfusetopentBipyr_Re_v5_C2_e	-552.95048350	61.61	
271	4-Icos-1vx_Re_v5c_C2_v	-552.95042034	61.65	
272	2-TricapCubeA_Re_v4b_C2_n	-552.94997145	61.93	
273	4-Icos-1vx_Re_v5c_C2_j	-552.94997145	61.93	
274	2-TricapCubeA_Re_v4b_C2_s	-552.94997142	61.93	
275	4-Icos-1vx_Re_v5c_C2_z	-552.94990602	61.97	
276	3-OhfusetopentBipyr_Re_v4_C2_a	-552.94988211	61.99	C-C
277	4-Icos-1vx_Re_v5b_C2_d	-552.94966548	62.13	
278	3-OhfusetopentBipyr_Re_v4_C2_s	-552.94933419	62.33	C-C
279	2-TricapCubeA_Re_v4b_C2_k	-552.94881879	62.66	
280	2-TricapCubeA_Re_v4b_C2_c	-552.94881875	62.66	
281	4-Icos-1vx_Re_v5c_C2_u	-552.94881874	62.66	
282	4-Icos-1vx_Re_v5c_C2_w	-552.94881874	62.66	
283	2-TricapCubeB_Re_v6_C2_p	-552.94874666	62.70	C-C
284	1-PentaCapTrPr_Re_v3_C2_v63b	-552.94874664	62.70	C-C

285	4-Icos-1vx_Re_v5a_C2_n	-552.94860902	62.79	
286	4-Icos-1vx_Re_v5c_C2_c	-552.94853087	62.84	
287	3-OhfusetopentBipyr_Re_v6b_C2dr-167	-552.94795443	63.20	
288	3-OhfusetopentBipyr_Re_v6b_C2kr-167	-552.94795443	63.20	
289	3-OhfusetopentBipyr_Re_v4_C2_k	-552.94795442	63.20	
290	2-TricapCubeB_Re_v6_C2_a	-552.94771747	63.35	C-C
291	4-Icos-1vx_Re_v5b_C2_c	-552.94733733	63.59	C-C
292	2-TricapCubeB_Re_v4_C2_p	-552.94733728	63.59	C-C
293	4-Icos-1vx_Re_v4_C2_m	-552.94733728	63.59	C-C
294	4-Icos-1vx_Re_v5c_C2_g	-552.94733728	63.59	C-C
295	1-PentacapTrPr_Re_v6_C2_i	-552.94722947	63.65	
296	3-OhfusetopentBipyr_Re_v4_C2_t	-552.94560104	64.68	
297	3-OhfusetopentBipyr_Re_v6b_C2_t	-552.94560104	64.68	
298	3-OhfusetopentBipyr_Re_v6b_C2_g	-552.94558353	64.69	C-C
299	3-OhfusetopentBipyr_Re_v6a_C2_d	-552.94558352	64.69	C-C
300	4-Icos-1vx_Re_v5a_C2_t	-552.94407574	65.63	C-C
301	4-Icos-1vx_Re_v5c_C2_s	-552.94302640	66.29	C-C
302	4-Icos-1vx_Re_v5a_C2_z	-552.94261925	66.55	C-C
303	3-OhfusetopentBipyr_Re_v6a_C2_s_r-31	-552.94255614	66.59	C-C
304	3-OhfusetopentBipyr_Re_v5_C2_c	-552.94243591	66.66	
305	2-TricapCubeB_Re_v4_C2_o	-552.94224310	66.78	C-C
306	3-OhfusetopentBipyr_Re_v6a_C2_a	-552.94183325	67.04	
307	4-Icos-1vx_Re_v4_C2_e	-552.94155064	67.22	
308	2-TricapCubeB_Re_v4_C2_l	-552.94138885	67.32	
309	3-OhfusetopentBipyr_Re_v6a_C2_s_i-31	-552.94074778	67.72	C-C
310	3-OhfusetopentBipyr_Re_v6b_C2_n	-552.94059746	67.82	C-C
311	2-TricapCubeB_Re_v6_C2_t	-552.94046776	67.90	
312	3-OhfusetopentBipyr_Re_v6b_C2_ir-100	-552.93899353	68.82	
313	3-OhfusetopentBipyr_Re_v6b_C2_o	-552.93899353	68.82	
314	3-OhfusetopentBipyr_Re_v6b_C2_i_r-25	-552.93899351	68.82	
315	4-Icos-1vx_Re_v5c_C2_i	-552.93883474	68.92	
316	4-Icos-1vx_Re_v5b_C2_m	-552.93752100	69.75	
317	2-TricapCubeA_Re_v4b_C2_v	-552.93746651	69.78	C-C
318	3-OhfusetopentBipyr_Re_v6b_C2_i_imag	-552.93699163	70.08	
319	3-OhfusetopentBipyr_Re_v5_C2_y	-552.93690613	70.13	
320	4-Icos-1vx_Re_v5c_C2_l	-552.93642252	70.44	C-C
321	4-Icos-1vx_Re_v5a_C2_zj	-552.93642251	70.44	C-C
322	3-OhfusetopentBipyr_Re_v5_C2_z	-552.93540228	71.08	

323	2-TricapCubeA_Re_v4b_C2_g	-552.93514805	71.24	C-C
324	4-Icos-1vx_Re_v4_C2_g	-552.93514805	71.24	C-C
325	2-TricapCubeA_Re_v4b_C2_e	-552.93497834	71.34	
326	3-OhfusetopentBipyr_Re_v6b_C2_m	-552.93443008	71.69	C-C
327	3-OhfusetopentBipyr_Re_v6b_C2_x	-552.93443008	71.69	C-C
328	4-Icos-1vx_Re_v5a_C2_zf	-552.93429231	71.77	C-C
329	4-Icos-1vx_Re_v5a_C2_zi_631Gd	-552.93388604	72.03	
330	3-OhfusetopentBipyr_Re_v6b_C2_z	-552.93380785	72.08	
331	3-OhfusetopentBipyr_Re_v4_C2_o	-552.93373072	72.12	
332	3-OhfusetopentBipyr_Re_v5_C2_a	-552.93317121	72.48	C-C
333	2-TricapCubeA_Re_v4b_C2_f	-552.93295655	72.61	C-C
334	4-Icos-1vx_Re_v5b_C2_b	-552.93295653	72.61	C-C
335	3-OhfusetopentBipyr_Re_v6b_C2_l	-552.93200914	73.20	
336	3-OhfusetopentBipyr_Re_v6b_C2_y	-552.93200914	73.20	
337	3-OhfusetopentBipyr_Re_v6b_C2_u	-552.93162235	73.45	C-C
338	3-OhfusetopentBipyr_Re_v5_C2_w	-552.93162234	73.45	C-C
339	3-OhfusetopentBipyr_Re_v6b_C2_r	-552.93162232	73.45	C-C
340	3-OhfusetopentBipyr_Re_v4_C2_w	-552.92926444	74.93	
341	3-OhfusetopentBipyr_Re_v4_C2_e	-552.92880810	75.21	
342	3-OhfusetopentBipyr_Re_v6b_C2_e	-552.92880810	75.21	
343	4-Icos-1vx_Re_v5c_C2_e	-552.92737342	76.11	C-C
344	2-TricapCubeA_Re_v4b_C2_u	-552.92734540	76.13	C-C
345	3-OhfusetopentBipyr_Re_v6b_C2_c	-552.92688053	76.42	
346	3-OhfusetopentBipyr_Re_v6b_C2_pr131	-552.92688050	76.42	
347	3-OhfusetopentBipyr_Re_v5_C2_h	-552.92613404	76.89	C-C
348	3-OhfusetopentBipyr_Re_v6b_C2_h	-552.92608706	76.92	C-C
349	3-OhfusetopentBipyr_Re_v6b_C2_s	-552.92608696	76.92	C-C
350	3-OhfusetopentBipyr_Re_v5_C2_r	-552.92483262	77.71	C-C
351	4-Icos-1vx_Re_v5a_C2_y	-552.92446869	77.94	
352	3-OhfusetopentBipyr_Re_v6b_C2_ki-167	-552.92445011	77.95	
353	3-OhfusetopentBipyr_Re_v6b_C2di-167	-552.92445010	77.95	
354	4-Icos-1vx_Re_v5b_C2_i	-552.92098095	80.13	C-C
355	2-TricapCubeB_Re_v4_C2_w	-552.92061405	80.36	
356	4-Icos-1vx_Re_v5c_C2_b	-552.91995006	80.77	C-C
357	4-Icos-1vx_Re_v4_C2_p	-552.91820895	81.86	C-C
358	3-OhfusetopentBipyr_Re_v4_C2_p	-552.91764356	82.22	
359	4-Icos-1vx_Re_v5b_C2_j	-552.91685648	82.71	
360	3-OhfusetopentBipyr_Re_v6b_C2_a	-552.91653678	82.91	C-C
361	3-OhfusetopentBipyr_Re_v6b_C2_w_r-182	-552.91653677	82.91	C-C

362	2-TricapCubeA_Re_v4b_C2_y	-552.91641420	82.99	C-C
363	3-OhfusetopentBipyr_Re_v5_C2_n	-552.91588675	83.32	
364	2-TricapCubeA_Re_v4b_C2_b	-552.91462260	84.11	C-C
365	2-TricapCubeA_Re_v4b_C2_p	-552.91462260	84.11	
366	3-OhfusetopentBipyr_Re_v6a_C2_w	-552.91444179	84.23	C-C
367	4-Icos-1vx_Re_v5c_C2_p	-552.91417600	84.40	C-C
368	3-OhfusetopentBipyr_Re_v6b_C2_p i-131	-552.91346834	84.84	
369	2-TricapCubeB_Re_v4_C2_n	-552.91307181	85.09	
370	4-Icos-1vx_Re_v5b_C2_x	-552.91307013	85.09	C-C
371	2-TricapCubeA_Re_v4b_C2_r	-552.91289276	85.20	C-C
372	4-Icos-1vx_Re_v5c_C2_t	-552.91207094	85.72	C-C
373	3-OhfusetopentBipyr_Re_v5_C2_d	-552.91096567	86.41	C-C
374	3-OhfusetopentBipyr_Re_v5_C2_l	-552.91096567	86.41	C-C
375	3-OhfusetopentBipyr_Re_v4_C2_n	-552.91093070	86.43	C-C
376	3-OhfusetopentBipyr_Re_v5_C2_x	-552.91018458	86.90	C-C
377	4-Icos-1vx_Re_v4_C2_v	-552.90976014	87.17	C-C
378	3-OhfusetopentBipyr_Re_v6a_C2_i	-552.90788251	88.34	C-C
379	2-TricapCubeB_Re_v4_C2_x	-552.90778665	88.40	C-C
380	3-OhfusetopentBipyr_Re_v4_C2_f	-552.90768411	88.47	C-C
381	3-OhfusetopentBipyr_Re_v6a_C2_hi-109	-552.90737064	88.67	
382	4-Icos-1vx_Re_v4_C2_j	-552.90554339	89.81	C-C
383	3-OhfusetopentBipyr_Re_v5_C2_q	-552.90381505	90.90	C-C
384	4-Icos-1vx_Re_v4_C2_r	-552.90329644	91.22	C-C
385	3-OhfusetopentBipyr_Re_v4_C2_q	-552.89985297	93.38	
386	3-OhfusetopentBipyr_Re_v6b_C2_zc	-552.89841506	94.29	
387	3-OhfusetopentBipyr_Re_v6b_C2_zd	-552.89547784	96.13	
388	3-OhfusetopentBipyr_Re_v6a_C2_z	-552.89382428	97.17	
389	3-OhfusetopentBipyr_Re_v4_C2_v	-552.88972425	99.74	C-C
390	3-OhfusetopentBipyr_Re_v4_C2_b	-552.88965327	99.78	
391	3-OhfusetopentBipyr_Re_v6b_C2_wi182	-552.88801468	100.81	C-C
392	2-TricapCubeB_Re_v6_C2_i	-552.88799585	100.82	C-C
393	1-PentaCapTrPr_Re_v6_C2_g	-552.88162634	104.82	C-C
394	3-OhfusetopentBipyr_Re_v6b_C2_ze	-552.88102975	105.19	
395	3-OhfusetopentBipyr_Re_v4_C2_g	-552.86678022	114.14	
396	3-OhfusetopentBipyr_Re_v4_C2_l	-552.85988480	118.46	C-C
397	3-OhfusetopentBipyr_Re_v4_C2_m	-552.84449662	128.12	
398	3-OhfusetopentBipyr_Re_v4_C2_h	-552.84352002	128.73	C-C

12-vertex $\text{CpMnC}_2\text{B}_9\text{H}_{11}$

Table 1. Initial structures (one example from each family) 128 structures in total

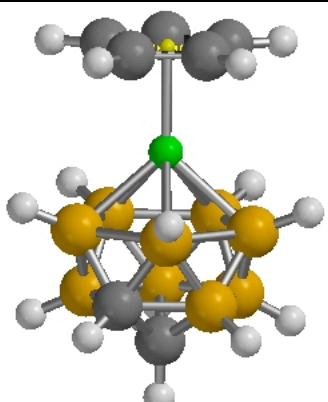
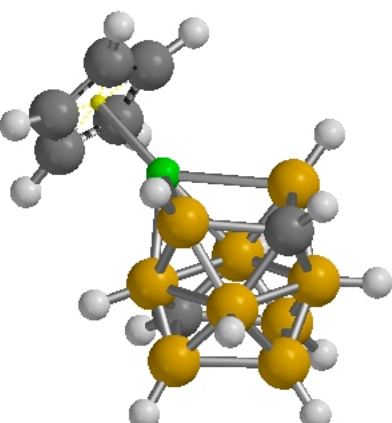
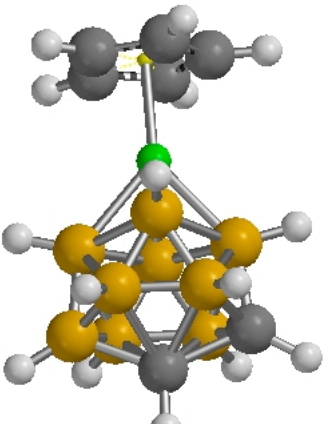
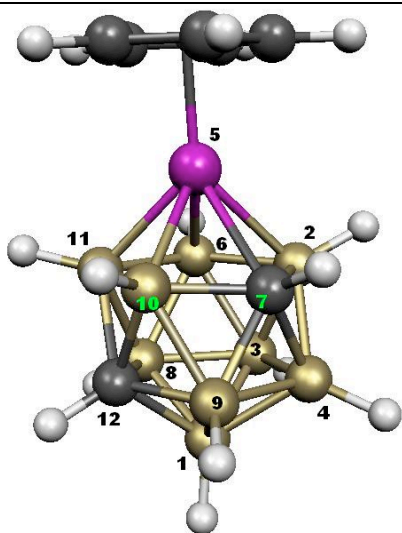
Initial structures
 <p>1. Icosahedron 9 structures</p>
 <p>2. Cubeoctahedron 49 structures</p>
 <p>3. Anticubeoctahedron 70 structures</p>

Table 3. Distance table for the best structures

	<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>2.907516</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.792601</td><td>1.805701</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.772187</td><td>1.789125</td><td>1.761497</td><td>0.000000</td><td></td></tr> <tr><td>5 Mn</td><td>3.981172</td><td>2.110174</td><td>3.373148</td><td>3.396826</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.907603</td><td>1.814500</td><td>1.805804</td><td>2.894749</td><td>2.110057</td></tr> <tr><td>7 C</td><td>2.775508</td><td>1.693510</td><td>2.765260</td><td>1.723657</td><td>2.127889</td></tr> <tr><td>8 B</td><td>1.772238</td><td>2.894747</td><td>1.761523</td><td>2.853900</td><td>3.396860</td></tr> <tr><td>9 B</td><td>1.784866</td><td>2.868477</td><td>2.876908</td><td>1.782406</td><td>3.396443</td></tr> <tr><td>10 C</td><td>2.775577</td><td>2.780745</td><td>2.765313</td><td>3.259158</td><td>2.127822</td></tr> <tr><td>11 B</td><td>1.784892</td><td>3.388030</td><td>2.876892</td><td>2.879173</td><td>3.396433</td></tr> <tr><td>12 B</td><td>2.839236</td><td>2.801109</td><td>3.314271</td><td>2.835461</td><td>2.126322</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 C</td><td>2.780714</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.789235</td><td>3.259188</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.388043</td><td>1.702916</td><td>2.879189</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>1.693502</td><td>2.680900</td><td>1.723769</td><td>2.775365</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.868461</td><td>2.775396</td><td>1.782378</td><td>1.791500</td><td>1.702906</td></tr> <tr><td>12 B</td><td>2.801064</td><td>1.682374</td><td>2.835505</td><td>1.757328</td><td>1.682327</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.757357</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.907516	0.000000				3 B	1.792601	1.805701	0.000000			4 B	1.772187	1.789125	1.761497	0.000000		5 Mn	3.981172	2.110174	3.373148	3.396826	0.000000	6 B	2.907603	1.814500	1.805804	2.894749	2.110057	7 C	2.775508	1.693510	2.765260	1.723657	2.127889	8 B	1.772238	2.894747	1.761523	2.853900	3.396860	9 B	1.784866	2.868477	2.876908	1.782406	3.396443	10 C	2.775577	2.780745	2.765313	3.259158	2.127822	11 B	1.784892	3.388030	2.876892	2.879173	3.396433	12 B	2.839236	2.801109	3.314271	2.835461	2.126322		6	7	8	9	10	6 B	0.000000					7 C	2.780714	0.000000				8 B	1.789235	3.259188	0.000000			9 B	3.388043	1.702916	2.879189	0.000000		10 C	1.693502	2.680900	1.723769	2.775365	0.000000	11 B	2.868461	2.775396	1.782378	1.791500	1.702906	12 B	2.801064	1.682374	2.835505	1.757328	1.682327		11	12				11 B	0.000000					12 B	1.757357	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	2.907516	0.000000																																																																																																																																															
3 B	1.792601	1.805701	0.000000																																																																																																																																														
4 B	1.772187	1.789125	1.761497	0.000000																																																																																																																																													
5 Mn	3.981172	2.110174	3.373148	3.396826	0.000000																																																																																																																																												
6 B	2.907603	1.814500	1.805804	2.894749	2.110057																																																																																																																																												
7 C	2.775508	1.693510	2.765260	1.723657	2.127889																																																																																																																																												
8 B	1.772238	2.894747	1.761523	2.853900	3.396860																																																																																																																																												
9 B	1.784866	2.868477	2.876908	1.782406	3.396443																																																																																																																																												
10 C	2.775577	2.780745	2.765313	3.259158	2.127822																																																																																																																																												
11 B	1.784892	3.388030	2.876892	2.879173	3.396433																																																																																																																																												
12 B	2.839236	2.801109	3.314271	2.835461	2.126322																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 C	2.780714	0.000000																																																																																																																																															
8 B	1.789235	3.259188	0.000000																																																																																																																																														
9 B	3.388043	1.702916	2.879189	0.000000																																																																																																																																													
10 C	1.693502	2.680900	1.723769	2.775365	0.000000																																																																																																																																												
11 B	2.868461	2.775396	1.782378	1.791500	1.702906																																																																																																																																												
12 B	2.801064	1.682374	2.835505	1.757328	1.682327																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.757357	0.000000																																																																																																																																															
	<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>2.880932</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.776183</td><td>1.771996</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.779371</td><td>1.790149</td><td>1.768359</td><td>0.000000</td><td></td></tr> <tr><td>5 Mn</td><td>3.952291</td><td>2.131515</td><td>3.405456</td><td>3.349987</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.741860</td><td>1.692036</td><td>1.696298</td><td>2.746308</td><td>2.174345</td></tr> <tr><td>7 B</td><td>2.925301</td><td>1.805267</td><td>2.911754</td><td>1.804154</td><td>2.076617</td></tr> <tr><td>8 B</td><td>1.776570</td><td>2.869835</td><td>1.799820</td><td>2.876356</td><td>3.404299</td></tr> <tr><td>9 C</td><td>1.692238</td><td>2.747329</td><td>2.731706</td><td>1.684468</td><td>3.218388</td></tr> <tr><td>10 B</td><td>2.881926</td><td>2.836306</td><td>2.872740</td><td>3.364819</td><td>2.133286</td></tr> <tr><td>11 B</td><td>1.780619</td><td>3.361501</td><td>2.877346</td><td>2.858808</td><td>3.347452</td></tr> <tr><td>12 B</td><td>2.927826</td><td>2.892346</td><td>3.425069</td><td>2.900935</td><td>2.075649</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.798700</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.693765</td><td>3.422359</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.079278</td><td>1.741700</td><td>2.732778</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.692118</td><td>2.892971</td><td>1.771706</td><td>2.750334</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.744792</td><td>2.895575</td><td>1.770530</td><td>1.685445</td><td>1.788900</td></tr> <tr><td>12 B</td><td>2.798610</td><td>1.800913</td><td>2.912507</td><td>1.746432</td><td>1.805572</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.802190</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.880932	0.000000				3 B	1.776183	1.771996	0.000000			4 B	1.779371	1.790149	1.768359	0.000000		5 Mn	3.952291	2.131515	3.405456	3.349987	0.000000	6 C	2.741860	1.692036	1.696298	2.746308	2.174345	7 B	2.925301	1.805267	2.911754	1.804154	2.076617	8 B	1.776570	2.869835	1.799820	2.876356	3.404299	9 C	1.692238	2.747329	2.731706	1.684468	3.218388	10 B	2.881926	2.836306	2.872740	3.364819	2.133286	11 B	1.780619	3.361501	2.877346	2.858808	3.347452	12 B	2.927826	2.892346	3.425069	2.900935	2.075649		6	7	8	9	10	6 C	0.000000					7 B	2.798700	0.000000				8 B	1.693765	3.422359	0.000000			9 C	3.079278	1.741700	2.732778	0.000000		10 B	1.692118	2.892971	1.771706	2.750334	0.000000	11 B	2.744792	2.895575	1.770530	1.685445	1.788900	12 B	2.798610	1.800913	2.912507	1.746432	1.805572		11	12				11 B	0.000000					12 B	1.802190	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	2.880932	0.000000																																																																																																																																															
3 B	1.776183	1.771996	0.000000																																																																																																																																														
4 B	1.779371	1.790149	1.768359	0.000000																																																																																																																																													
5 Mn	3.952291	2.131515	3.405456	3.349987	0.000000																																																																																																																																												
6 C	2.741860	1.692036	1.696298	2.746308	2.174345																																																																																																																																												
7 B	2.925301	1.805267	2.911754	1.804154	2.076617																																																																																																																																												
8 B	1.776570	2.869835	1.799820	2.876356	3.404299																																																																																																																																												
9 C	1.692238	2.747329	2.731706	1.684468	3.218388																																																																																																																																												
10 B	2.881926	2.836306	2.872740	3.364819	2.133286																																																																																																																																												
11 B	1.780619	3.361501	2.877346	2.858808	3.347452																																																																																																																																												
12 B	2.927826	2.892346	3.425069	2.900935	2.075649																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 C	0.000000																																																																																																																																																
7 B	2.798700	0.000000																																																																																																																																															
8 B	1.693765	3.422359	0.000000																																																																																																																																														
9 C	3.079278	1.741700	2.732778	0.000000																																																																																																																																													
10 B	1.692118	2.892971	1.771706	2.750334	0.000000																																																																																																																																												
11 B	2.744792	2.895575	1.770530	1.685445	1.788900																																																																																																																																												
12 B	2.798610	1.800913	2.912507	1.746432	1.805572																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.802190	0.000000																																																																																																																																															

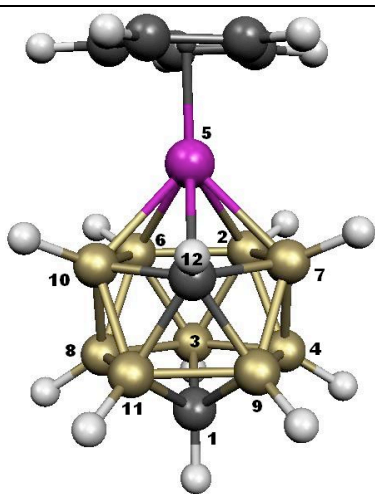
1. -1651.06958759 Cs 0.0

2. -1651.06958620 Cs 0.0



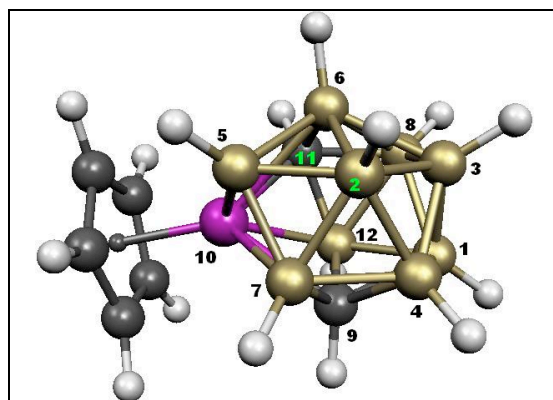
3. -1651.06538765 +2.6

	1	2	3	4	5
1 B	0.000000				
2 B	2.864258	0.000000			
3 B	1.783761	1.786964	0.000000		
4 B	1.779026	1.760950	1.793170	0.000000	
5 Mn	3.952439	2.154052	3.367634	3.409748	0.000000
6 B	2.921782	1.811006	1.796860	2.920443	2.103484
7 C	2.755212	1.693863	2.772455	1.703042	2.166684
8 B	1.767305	2.869403	1.762520	2.868712	3.338465
9 B	1.768505	2.839111	2.871227	1.775694	3.384573
10 B	2.895380	2.818274	3.372270	2.870864	2.090066
11 B	2.930268	2.898379	2.911608	3.432259	2.075033
12 C	1.705330	3.199885	2.738793	2.745557	3.222756
	6	7	8	9	10
6 B	0.000000				
7 C	2.814776	0.000000			
8 B	1.810835	3.242093	0.000000		
9 B	3.411195	1.688356	2.848132	0.000000	
10 B	2.888592	1.683057	2.878009	1.787032	0.000000
11 B	1.817577	2.806220	1.818394	2.904010	1.794579
12 C	2.776431	2.619910	1.687358	1.687349	1.728157
	11	12			
11 B	0.000000				
12 C	1.733514	0.000000			



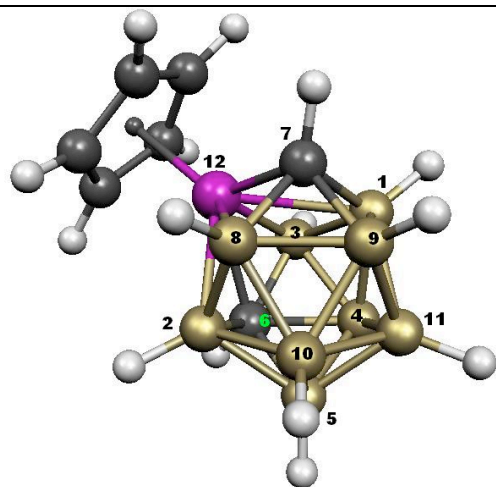
4. -1651.06340365 Cs +3.9

	1	2	3	4	5
1 C	0.000000				
2 B	2.793424	0.000000			
3 B	1.695948	1.810088	0.000000		
4 B	1.709564	1.788891	1.764007	0.000000	
5 Mn	3.785535	2.091650	3.327713	3.341539	0.000000
6 B	2.791633	1.829921	1.807717	2.906050	2.091344
7 B	2.752294	1.816937	2.885950	1.793447	2.131312
8 B	1.708477	2.909413	1.763228	2.870391	3.343372
9 B	1.700681	2.896034	2.856435	1.769557	3.374676
10 B	2.751871	2.917124	2.883958	3.374665	2.129474
11 B	1.700451	3.418013	2.855480	2.880331	3.375293
12 C	2.615413	2.820139	3.243663	2.759749	2.168761
	6	7	8	9	10
6 B	0.000000				
7 B	2.917422	0.000000			
8 B	1.790111	3.376823	0.000000		
9 B	3.415762	1.751383	2.879382	0.000000	
10 B	1.814939	2.848677	1.794774	2.861709	0.000000
11 B	2.894245	2.863585	1.767539	1.799689	1.751767
12 C	2.819151	1.699323	2.760884	1.683351	1.699535
	11	12			
11 B	0.000000				
12 C	1.685326	0.000000			



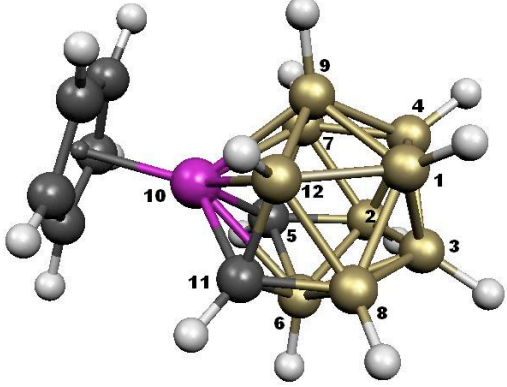
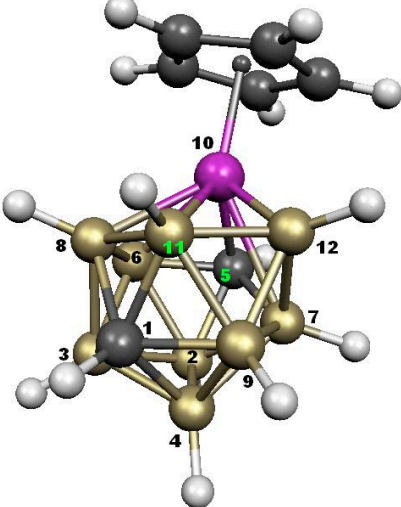
5. -1651.06102929 +5.4

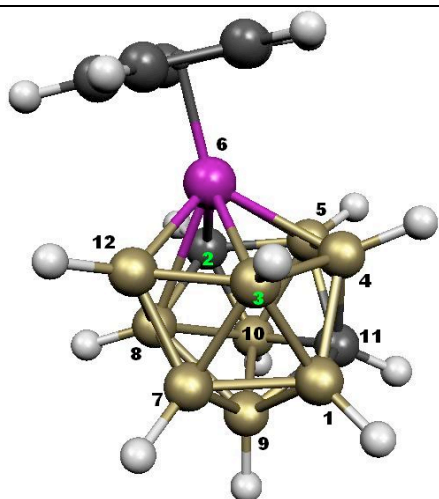
	1	2	3	4	5
1 B	0.000000				
2 B	2.884769	0.000000			
3 B	1.765722	1.755160	0.000000		
4 B	1.730279	1.765952	1.747870	0.000000	
5 B	3.741764	1.731325	3.061871	2.953349	0.000000
6 B	2.877259	1.909525	1.914451	2.891898	1.956391
7 B	2.902166	1.809897	2.870921	1.799636	1.739345
8 B	1.772145	3.049529	1.782869	2.913178	3.562783
9 C	1.738914	2.698930	2.686563	1.741845	2.876366
10 Mn	3.289447	3.002040	3.492561	3.289134	1.944728
11 C	2.743588	3.222787	2.800579	3.488209	2.874440
12 B	1.808126	3.492282	2.871852	2.912154	3.471252
	6	7	8	9	10
6 B	0.000000				
7 B	2.788684	0.000000			
8 B	1.927869	3.572482	0.000000		
9 C	2.953370	1.655266	2.756678	0.000000	
10 Mn	2.379532	2.157905	3.092611	2.132681	0.000000
11 C	1.672273	3.290679	1.604134	2.709592	1.901980
12 B	2.725088	3.004329	1.834919	1.677614	2.147191
	11	12			
11 C	0.000000				
12 B	1.623236	0.000000			



6. -1651.06040132 +5.8

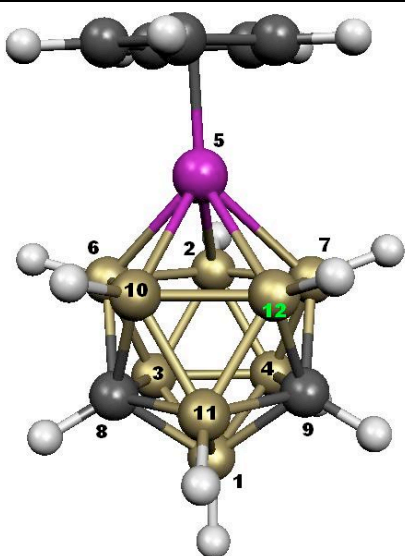
	1	2	3	4	5
1 B	0.000000				
2 B	3.089909	0.000000			
3 B	1.933133	2.904322	0.000000		
4 B	1.886220	2.807929	1.752834	0.000000	
5 B	2.914911	1.833374	2.931729	1.762085	0.000000
6 C	2.655691	1.662554	1.643333	1.711168	1.714987
7 C	1.679561	2.804486	2.862457	3.201183	3.489996
8 B	2.757153	1.781870	3.479505	3.504750	2.942848
9 B	1.969560	2.892140	3.557775	3.017553	2.919889
10 B	2.916847	1.831515	3.717379	2.870507	1.738978
11 B	1.945698	2.829537	3.060650	1.724914	1.761933
12 Mn	2.357208	2.152596	1.915191	3.003973	3.286029
	6	7	8	9	10
6 C	0.000000				
7 C	3.194663	0.000000			
8 B	2.982572	1.620223	0.000000		
9 B	3.456738	1.608269	1.822509	0.000000	
10 B	2.805437	2.736623	1.793622	1.780823	0.000000
11 B	2.743136	2.789630	2.872933	1.769134	1.782651
12 Mn	2.131853	1.894685	2.176776	3.091101	3.269959
	11	12			
11 B	0.000000				
12 Mn	3.484039	0.000000			

 <p>7. -1651.05958737 Cs +6.3</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>2.924551</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.755039</td><td>1.764720</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.744000</td><td>1.803699</td><td>1.755039</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>3.515461</td><td>1.596899</td><td>2.841690</td><td>2.749169</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.925009</td><td>1.932568</td><td>1.993592</td><td>2.925009</td><td>1.718298</td></tr> <tr><td>7 B</td><td>2.940883</td><td>1.866013</td><td>2.890179</td><td>1.813692</td><td>1.615748</td></tr> <tr><td>8 B</td><td>1.803699</td><td>3.038800</td><td>1.764720</td><td>2.924551</td><td>3.303738</td></tr> <tr><td>9 B</td><td>1.812183</td><td>2.892213</td><td>2.814714</td><td>1.812183</td><td>2.826524</td></tr> <tr><td>10 Mn</td><td>3.287153</td><td>3.069858</td><td>3.500099</td><td>3.287153</td><td>1.896892</td></tr> <tr><td>11 C</td><td>2.749237</td><td>3.303745</td><td>2.841705</td><td>3.515514</td><td>2.752600</td></tr> <tr><td>12 B</td><td>1.813692</td><td>3.580536</td><td>2.890179</td><td>2.940883</td><td>3.327068</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.767671</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.932568</td><td>3.580536</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.108025</td><td>1.761382</td><td>2.892213</td><td>0.000000</td><td></td></tr> <tr><td>10 Mn</td><td>2.333537</td><td>2.171662</td><td>3.069858</td><td>2.208356</td><td>0.000000</td></tr> <tr><td>11 C</td><td>1.718259</td><td>3.327116</td><td>1.596913</td><td>2.826610</td><td>1.896934</td></tr> <tr><td>12 B</td><td>2.767671</td><td>3.073000</td><td>1.866013</td><td>1.761382</td><td>2.171662</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.615846</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.924551	0.000000				3 B	1.755039	1.764720	0.000000			4 B	1.744000	1.803699	1.755039	0.000000		5 C	3.515461	1.596899	2.841690	2.749169	0.000000	6 B	2.925009	1.932568	1.993592	2.925009	1.718298	7 B	2.940883	1.866013	2.890179	1.813692	1.615748	8 B	1.803699	3.038800	1.764720	2.924551	3.303738	9 B	1.812183	2.892213	2.814714	1.812183	2.826524	10 Mn	3.287153	3.069858	3.500099	3.287153	1.896892	11 C	2.749237	3.303745	2.841705	3.515514	2.752600	12 B	1.813692	3.580536	2.890179	2.940883	3.327068		6	7	8	9	10	6 B	0.000000					7 B	2.767671	0.000000				8 B	1.932568	3.580536	0.000000			9 B	3.108025	1.761382	2.892213	0.000000		10 Mn	2.333537	2.171662	3.069858	2.208356	0.000000	11 C	1.718259	3.327116	1.596913	2.826610	1.896934	12 B	2.767671	3.073000	1.866013	1.761382	2.171662		11	12				11 C	0.000000					12 B	1.615846	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	2.924551	0.000000																																																																																																																																															
3 B	1.755039	1.764720	0.000000																																																																																																																																														
4 B	1.744000	1.803699	1.755039	0.000000																																																																																																																																													
5 C	3.515461	1.596899	2.841690	2.749169	0.000000																																																																																																																																												
6 B	2.925009	1.932568	1.993592	2.925009	1.718298																																																																																																																																												
7 B	2.940883	1.866013	2.890179	1.813692	1.615748																																																																																																																																												
8 B	1.803699	3.038800	1.764720	2.924551	3.303738																																																																																																																																												
9 B	1.812183	2.892213	2.814714	1.812183	2.826524																																																																																																																																												
10 Mn	3.287153	3.069858	3.500099	3.287153	1.896892																																																																																																																																												
11 C	2.749237	3.303745	2.841705	3.515514	2.752600																																																																																																																																												
12 B	1.813692	3.580536	2.890179	2.940883	3.327068																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	2.767671	0.000000																																																																																																																																															
8 B	1.932568	3.580536	0.000000																																																																																																																																														
9 B	3.108025	1.761382	2.892213	0.000000																																																																																																																																													
10 Mn	2.333537	2.171662	3.069858	2.208356	0.000000																																																																																																																																												
11 C	1.718259	3.327116	1.596913	2.826610	1.896934																																																																																																																																												
12 B	2.767671	3.073000	1.866013	1.761382	2.171662																																																																																																																																												
	11	12																																																																																																																																															
11 C	0.000000																																																																																																																																																
12 B	1.615846	0.000000																																																																																																																																															
 <p>8. -1651.05821775 +7.1</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.791445</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.664690</td><td>1.783848</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.683576</td><td>1.753047</td><td>1.775951</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>3.326258</td><td>1.609272</td><td>2.730419</td><td>2.779758</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.811877</td><td>1.837101</td><td>1.792968</td><td>2.870116</td><td>1.622354</td></tr> <tr><td>7 B</td><td>2.747645</td><td>1.921439</td><td>2.879841</td><td>1.896301</td><td>1.680935</td></tr> <tr><td>8 B</td><td>1.755682</td><td>2.892668</td><td>1.823284</td><td>2.836086</td><td>2.796473</td></tr> <tr><td>9 B</td><td>1.691924</td><td>3.040804</td><td>2.889675</td><td>1.754805</td><td>3.224355</td></tr> <tr><td>10 Mn</td><td>3.124138</td><td>3.092559</td><td>3.261614</td><td>3.469981</td><td>1.897325</td></tr> <tr><td>11 B</td><td>1.714924</td><td>3.592786</td><td>2.915209</td><td>2.870684</td><td>3.310306</td></tr> <tr><td>12 B</td><td>2.819022</td><td>3.553248</td><td>3.727200</td><td>3.045051</td><td>2.873223</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.751875</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.764064</td><td>3.096143</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.532789</td><td>1.905169</td><td>2.841642</td><td>0.000000</td><td></td></tr> <tr><td>10 Mn</td><td>2.183861</td><td>2.380990</td><td>2.150624</td><td>3.001081</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.090895</td><td>2.790560</td><td>1.751188</td><td>1.795137</td><td>2.175106</td></tr> <tr><td>12 B</td><td>3.513071</td><td>1.950690</td><td>2.963182</td><td>1.725637</td><td>1.946432</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.718472</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	2.791445	0.000000				3 B	1.664690	1.783848	0.000000			4 B	1.683576	1.753047	1.775951	0.000000		5 C	3.326258	1.609272	2.730419	2.779758	0.000000	6 B	2.811877	1.837101	1.792968	2.870116	1.622354	7 B	2.747645	1.921439	2.879841	1.896301	1.680935	8 B	1.755682	2.892668	1.823284	2.836086	2.796473	9 B	1.691924	3.040804	2.889675	1.754805	3.224355	10 Mn	3.124138	3.092559	3.261614	3.469981	1.897325	11 B	1.714924	3.592786	2.915209	2.870684	3.310306	12 B	2.819022	3.553248	3.727200	3.045051	2.873223		6	7	8	9	10	6 B	0.000000					7 B	2.751875	0.000000				8 B	1.764064	3.096143	0.000000			9 B	3.532789	1.905169	2.841642	0.000000		10 Mn	2.183861	2.380990	2.150624	3.001081	0.000000	11 B	3.090895	2.790560	1.751188	1.795137	2.175106	12 B	3.513071	1.950690	2.963182	1.725637	1.946432		11	12				11 B	0.000000					12 B	1.718472	0.000000			
	1	2	3	4	5																																																																																																																																												
1 C	0.000000																																																																																																																																																
2 B	2.791445	0.000000																																																																																																																																															
3 B	1.664690	1.783848	0.000000																																																																																																																																														
4 B	1.683576	1.753047	1.775951	0.000000																																																																																																																																													
5 C	3.326258	1.609272	2.730419	2.779758	0.000000																																																																																																																																												
6 B	2.811877	1.837101	1.792968	2.870116	1.622354																																																																																																																																												
7 B	2.747645	1.921439	2.879841	1.896301	1.680935																																																																																																																																												
8 B	1.755682	2.892668	1.823284	2.836086	2.796473																																																																																																																																												
9 B	1.691924	3.040804	2.889675	1.754805	3.224355																																																																																																																																												
10 Mn	3.124138	3.092559	3.261614	3.469981	1.897325																																																																																																																																												
11 B	1.714924	3.592786	2.915209	2.870684	3.310306																																																																																																																																												
12 B	2.819022	3.553248	3.727200	3.045051	2.873223																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	2.751875	0.000000																																																																																																																																															
8 B	1.764064	3.096143	0.000000																																																																																																																																														
9 B	3.532789	1.905169	2.841642	0.000000																																																																																																																																													
10 Mn	2.183861	2.380990	2.150624	3.001081	0.000000																																																																																																																																												
11 B	3.090895	2.790560	1.751188	1.795137	2.175106																																																																																																																																												
12 B	3.513071	1.950690	2.963182	1.725637	1.946432																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.718472	0.000000																																																																																																																																															



9. -1651.05664731 +8.1

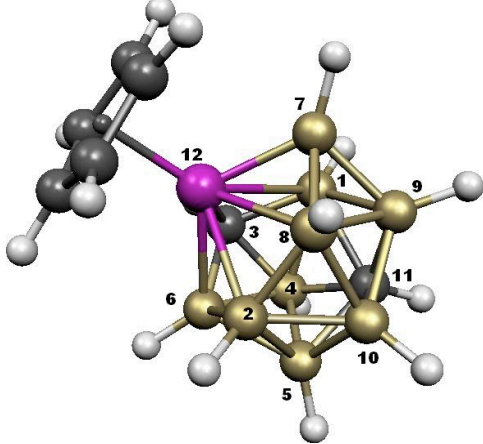
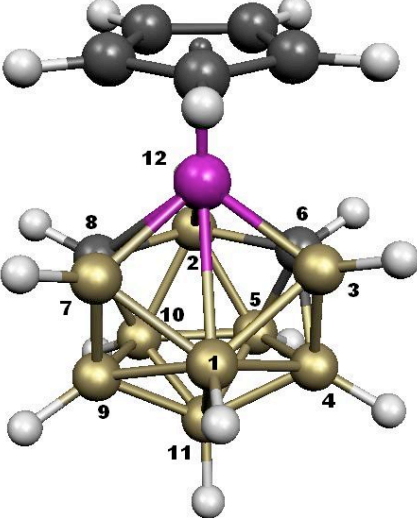
	1	2	3	4	5
1 B	0.000000				
2 C	3.481636	0.000000			
3 B	1.777144	3.347199	0.000000		
4 B	1.818275	2.821306	1.741505	0.000000	
5 B	2.915693	1.615840	3.086319	1.769145	0.000000
6 Mn	3.257767	1.901873	2.206029	2.156961	2.152739
7 B	1.778694	3.233130	1.802835	2.835819	3.517267
8 B	2.896373	1.673749	2.815615	3.099755	2.730425
9 B	1.764564	2.784097	2.865286	2.837399	2.872451
10 B	2.902806	1.599745	3.599872	2.894192	1.830228
11 C	1.666463	2.612686	2.811218	1.763793	1.726395
12 B	2.939924	2.900598	1.727461	2.954028	3.496848
	6	7	8	9	10
6 Mn	0.000000				
7 B	3.003173	0.000000			
8 B	2.369956	1.914812	0.000000		
9 B	3.460101	1.733926	1.893420	0.000000	
10 B	3.076393	3.036302	1.915827	1.763980	0.000000
11 C	3.127765	2.769818	2.737277	1.699731	1.692160
12 B	1.946027	1.740556	1.980201	3.047935	3.567178
	11	12			
11 C	0.000000				
12 B	3.593393	0.000000			

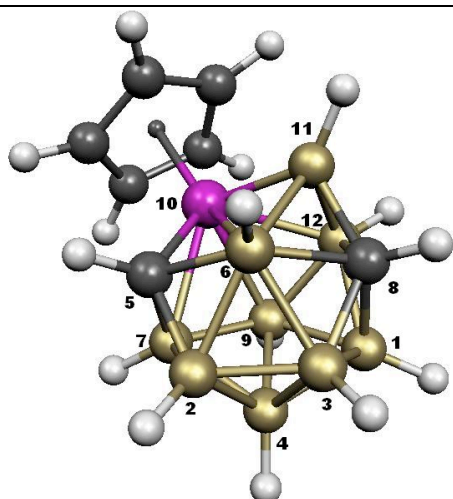


10. -1651.05572826 Cs +8.7

	1	2	3	4	5
1 B	0.000000				
2 B	2.883810	0.000000			
3 B	1.758446	1.806793	0.000000		
4 B	1.770504	1.769927	1.764177	0.000000	
5 Mn	3.931876	2.139432	3.350977	3.387501	0.000000
6 B	2.892482	1.819509	1.802174	2.892237	2.073610
7 B	2.853476	1.787625	2.877674	1.775294	2.199535
8 C	1.681275	2.780703	1.691118	2.736209	3.225090
9 C	1.698951	2.765728	2.747631	1.731630	3.273110
10 B	2.909639	2.934905	2.916640	3.420664	2.093032
11 B	1.788000	3.395111	2.861579	2.889673	3.345694
12 B	2.882634	2.917062	3.401084	2.905864	2.177380
	6	7	8	9	10
6 B	0.000000				
7 B	2.904879	0.000000			
8 C	1.735522	3.225838	0.000000		
9 C	3.251112	1.688903	2.601616	0.000000	
10 B	1.815616	2.902144	1.753976	2.763284	0.000000
11 B	2.874867	2.865370	1.678523	1.702554	1.770098
12 B	2.914801	1.793708	2.764156	1.698367	1.790962
	11	12			
11 B	0.000000				
12 B	1.770998	0.000000			

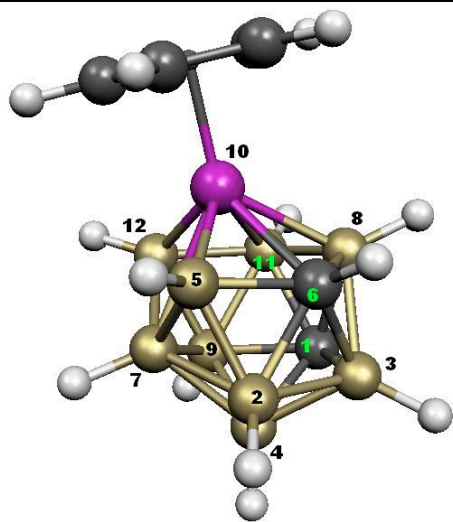
	1	2	3	4	5
1 B	0.000000				
2 B	3.089137	0.000000			
3 C	1.663844	2.834867	0.000000		
4 B	1.922441	2.891666	1.602045	0.000000	
5 B	2.888145	1.820451	2.741401	1.777891	0.000000
6 B	2.731638	1.786524	1.629642	1.825793	1.789234
7 B	1.921207	2.976716	2.883116	3.539913	3.736389

 <p>11. -1651.05281312 +10.5</p>	<table border="0"> <tbody> <tr><td>8 B</td><td>2.780169</td><td>1.760726</td><td>3.345821</td><td>3.590071</td><td>2.926757</td></tr> <tr><td>9 B</td><td>1.906789</td><td>2.844839</td><td>3.235706</td><td>3.023601</td><td>2.895450</td></tr> <tr><td>10 B</td><td>2.900835</td><td>1.813083</td><td>3.496057</td><td>2.908939</td><td>1.737347</td></tr> <tr><td>11 C</td><td>1.828333</td><td>2.684258</td><td>2.667429</td><td>1.686992</td><td>1.699308</td></tr> <tr><td>12 Mn</td><td>2.325998</td><td>2.175426</td><td>1.898441</td><td>3.067533</td><td>3.257241</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>3.513387</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.109958</td><td>1.733368</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.533019</td><td>1.738585</td><td>1.799301</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.932331</td><td>2.945575</td><td>1.776942</td><td>1.783539</td><td>0.000000</td></tr> <tr><td>11 C</td><td>2.733701</td><td>2.924567</td><td>2.732210</td><td>1.674762</td><td>1.691072</td></tr> <tr><td>12 Mn</td><td>2.179333</td><td>1.939236</td><td>2.199354</td><td>2.999434</td><td>3.257728</td></tr> <tr><td></td><td>11</td><td>12</td><td></td><td></td><td></td></tr> <tr><td>11 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Mn</td><td>3.298281</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>	8 B	2.780169	1.760726	3.345821	3.590071	2.926757	9 B	1.906789	2.844839	3.235706	3.023601	2.895450	10 B	2.900835	1.813083	3.496057	2.908939	1.737347	11 C	1.828333	2.684258	2.667429	1.686992	1.699308	12 Mn	2.325998	2.175426	1.898441	3.067533	3.257241		6	7	8	9	10	6 B	0.000000					7 B	3.513387	0.000000				8 B	3.109958	1.733368	0.000000			9 B	3.533019	1.738585	1.799301	0.000000		10 B	2.932331	2.945575	1.776942	1.783539	0.000000	11 C	2.733701	2.924567	2.732210	1.674762	1.691072	12 Mn	2.179333	1.939236	2.199354	2.999434	3.257728		11	12				11 C	0.000000					12 Mn	3.298281	0.000000																																																			
8 B	2.780169	1.760726	3.345821	3.590071	2.926757																																																																																																																																												
9 B	1.906789	2.844839	3.235706	3.023601	2.895450																																																																																																																																												
10 B	2.900835	1.813083	3.496057	2.908939	1.737347																																																																																																																																												
11 C	1.828333	2.684258	2.667429	1.686992	1.699308																																																																																																																																												
12 Mn	2.325998	2.175426	1.898441	3.067533	3.257241																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	3.513387	0.000000																																																																																																																																															
8 B	3.109958	1.733368	0.000000																																																																																																																																														
9 B	3.533019	1.738585	1.799301	0.000000																																																																																																																																													
10 B	2.932331	2.945575	1.776942	1.783539	0.000000																																																																																																																																												
11 C	2.733701	2.924567	2.732210	1.674762	1.691072																																																																																																																																												
12 Mn	2.179333	1.939236	2.199354	2.999434	3.257728																																																																																																																																												
	11	12																																																																																																																																															
11 C	0.000000																																																																																																																																																
12 Mn	3.298281	0.000000																																																																																																																																															
 <p>12. -1651.05214350 Cs +11.0</p>	<table border="0"> <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>3.076853</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.857160</td><td>2.884040</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.910445</td><td>2.822314</td><td>1.744943</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.907134</td><td>1.832097</td><td>2.907067</td><td>1.758997</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.645502</td><td>1.677671</td><td>1.648336</td><td>1.705435</td><td>1.704336</td></tr> <tr><td>7 B</td><td>1.856655</td><td>2.883287</td><td>2.891303</td><td>3.417305</td><td>3.668287</td></tr> <tr><td>8 C</td><td>2.645908</td><td>1.677590</td><td>3.317967</td><td>3.387410</td><td>2.806146</td></tr> <tr><td>9 B</td><td>1.911053</td><td>2.822870</td><td>3.418752</td><td>2.988406</td><td>2.877196</td></tr> <tr><td>10 B</td><td>2.907633</td><td>1.832244</td><td>3.669944</td><td>2.877283</td><td>1.734603</td></tr> <tr><td>11 B</td><td>1.915220</td><td>2.828402</td><td>2.992684</td><td>1.732391</td><td>1.781631</td></tr> <tr><td>12 Mn</td><td>2.416678</td><td>2.117170</td><td>1.922818</td><td>3.058605</td><td>3.281904</td></tr> <tr><td></td><td>6</td><td>7</td><td>8</td><td>9</td><td>10</td></tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.317015</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>2.867005</td><td>1.647943</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.388012</td><td>1.743628</td><td>1.705613</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.806904</td><td>2.905728</td><td>1.703576</td><td>1.759415</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.736299</td><td>2.991117</td><td>2.735864</td><td>1.732440</td><td>1.781995</td></tr> <tr><td>12 Mn</td><td>2.129585</td><td>1.921857</td><td>2.129015</td><td>3.058256</td><td>3.281644</td></tr> <tr><td></td><td>11</td><td>12</td><td></td><td></td><td></td></tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Mn</td><td>3.505087</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	3.076853	0.000000				3 B	1.857160	2.884040	0.000000			4 B	1.910445	2.822314	1.744943	0.000000		5 B	2.907134	1.832097	2.907067	1.758997	0.000000	6 C	2.645502	1.677671	1.648336	1.705435	1.704336	7 B	1.856655	2.883287	2.891303	3.417305	3.668287	8 C	2.645908	1.677590	3.317967	3.387410	2.806146	9 B	1.911053	2.822870	3.418752	2.988406	2.877196	10 B	2.907633	1.832244	3.669944	2.877283	1.734603	11 B	1.915220	2.828402	2.992684	1.732391	1.781631	12 Mn	2.416678	2.117170	1.922818	3.058605	3.281904		6	7	8	9	10	6 C	0.000000					7 B	3.317015	0.000000				8 C	2.867005	1.647943	0.000000			9 B	3.388012	1.743628	1.705613	0.000000		10 B	2.806904	2.905728	1.703576	1.759415	0.000000	11 B	2.736299	2.991117	2.735864	1.732440	1.781995	12 Mn	2.129585	1.921857	2.129015	3.058256	3.281644		11	12				11 B	0.000000					12 Mn	3.505087	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	3.076853	0.000000																																																																																																																																															
3 B	1.857160	2.884040	0.000000																																																																																																																																														
4 B	1.910445	2.822314	1.744943	0.000000																																																																																																																																													
5 B	2.907134	1.832097	2.907067	1.758997	0.000000																																																																																																																																												
6 C	2.645502	1.677671	1.648336	1.705435	1.704336																																																																																																																																												
7 B	1.856655	2.883287	2.891303	3.417305	3.668287																																																																																																																																												
8 C	2.645908	1.677590	3.317967	3.387410	2.806146																																																																																																																																												
9 B	1.911053	2.822870	3.418752	2.988406	2.877196																																																																																																																																												
10 B	2.907633	1.832244	3.669944	2.877283	1.734603																																																																																																																																												
11 B	1.915220	2.828402	2.992684	1.732391	1.781631																																																																																																																																												
12 Mn	2.416678	2.117170	1.922818	3.058605	3.281904																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 C	0.000000																																																																																																																																																
7 B	3.317015	0.000000																																																																																																																																															
8 C	2.867005	1.647943	0.000000																																																																																																																																														
9 B	3.388012	1.743628	1.705613	0.000000																																																																																																																																													
10 B	2.806904	2.905728	1.703576	1.759415	0.000000																																																																																																																																												
11 B	2.736299	2.991117	2.735864	1.732440	1.781995																																																																																																																																												
12 Mn	2.129585	1.921857	2.129015	3.058256	3.281644																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 Mn	3.505087	0.000000																																																																																																																																															



13. -1651.04959634 +12.5

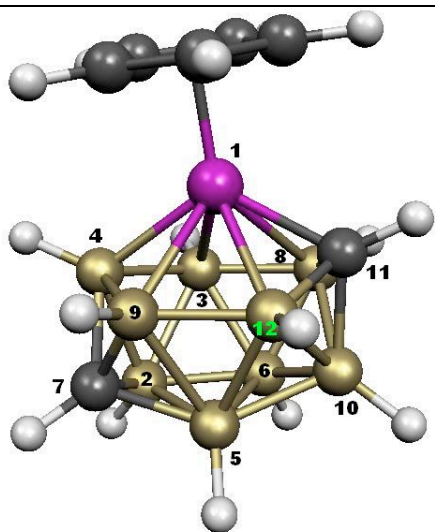
	1	2	3	4	5
1 B	0.000000				
2 B	2.929582	0.000000			
3 B	1.766172	1.768554	0.000000		
4 B	1.743799	1.794032	1.761835	0.000000	
5 C	3.478239	1.603874	2.798347	2.737283	0.000000
6 B	2.887689	1.901817	1.906599	2.874693	1.683158
7 B	2.927404	1.843590	2.872028	1.801677	1.619816
8 C	1.713419	2.906425	1.677877	2.775105	3.079107
9 B	1.819086	2.908555	2.834191	1.832529	2.813898
10 Mn	3.271536	3.097617	3.492150	3.293035	1.893618
11 B	2.906748	3.500604	3.008461	3.704592	2.836325
12 B	1.783244	3.582341	2.875934	2.918029	3.285589
	6	7	8	9	10
6 B	0.000000				
7 B	2.745176	0.000000			
8 C	1.791696	3.375868	0.000000		
9 B	3.111033	1.769523	2.729332	0.000000	
10 Mn	2.387637	2.192839	2.883608	2.197600	0.000000
11 B	1.903711	3.483250	1.640622	2.976323	1.947745
12 B	2.787536	3.056291	1.754749	1.734321	2.157753
	11	12			
11 B	0.000000				
12 B	1.730920	0.000000			



14. -1651.04637070 +14.6

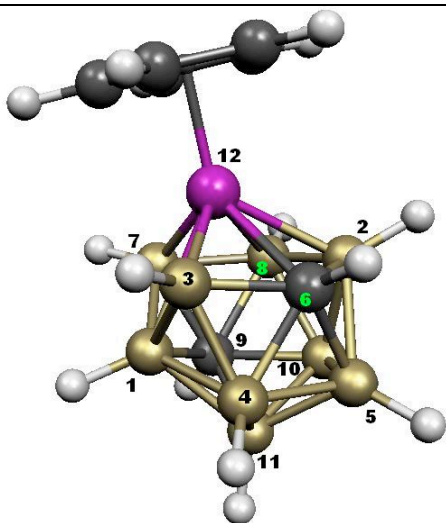
	1	2	3	4	5
1 C	0.000000				
2 B	2.756541	0.000000			
3 B	1.653523	1.754501	0.000000		
4 B	1.698358	1.729052	1.764229	0.000000	
5 B	3.503909	1.738560	2.886043	2.974522	0.000000
6 C	2.676503	1.719746	1.697211	2.734762	1.652900
7 B	2.753500	1.881504	2.866254	1.882235	1.844404
8 B	1.768604	2.843127	1.846275	2.847827	2.875963
9 B	1.694561	3.016405	2.880894	1.756740	3.424201
10 Mn	3.124624	3.065014	3.260315	3.490782	1.931309
11 B	1.715738	3.541340	2.917303	2.867046	3.434003
12 B	2.801925	3.429759	3.669814	2.984736	2.899517
	6	7	8	9	10
6 C	0.000000				
7 B	2.641701	0.000000			
8 B	1.670812	3.085611	0.000000		
9 B	3.409073	1.929412	2.851125	0.000000	
10 Mn	2.131429	2.433942	2.091312	3.049486	0.000000
11 B	2.987253	2.785217	1.761048	1.785589	2.173392
12 B	3.349389	1.876365	2.924098	1.725151	1.949724
	11	12			
11 B	0.000000				
12 B	1.722994	0.000000			

	1	2	3	4	5
1 Mn	0.000000				
2 B	3.339202	0.000000			
3 B	2.169980	1.871571	0.000000		
4 B	2.097951	1.922260	1.797994	0.000000	
5 B	3.204136	1.948276	2.842064	2.709027	0.000000
6 B	3.201146	1.743487	1.806973	2.918533	1.946054
7 C	3.150757	1.549111	2.732773	1.656368	1.691374



15. -1651.04534955 +15.2

8	B	2.289682	3.016218	1.775398	3.155302	2.937032
9	B	2.207894	2.711092	2.968970	1.815754	2.031534
10	B	3.008039	3.028174	2.882208	3.574762	1.826571
11	C	1.925998	3.738852	2.823986	3.429702	2.864972
12	B	2.178300	3.381713	3.201256	3.017538	1.987282
		6	7	8	9	10
6	B	0.000000				
7	C	2.791130	0.000000			
8	B	1.747315	3.696123	0.000000		
9	B	3.279744	1.563392	3.468009	0.000000	
10	B	1.768662	3.282555	1.839360	3.040659	0.000000
11	C	2.739304	3.777637	1.596929	2.944844	1.647552
12	B	2.963474	2.829475	2.691708	1.773798	1.815747
		11	12			
11	C	0.000000				
12	B	1.577416	0.000000			



16. -1651.04534255 +15.2

		1	2	3	4	5
1	B	0.000000				
2	B	3.100612	0.000000			
3	B	1.849760	2.893213	0.000000		
4	B	1.856081	2.848595	1.735574	0.000000	
5	B	2.872678	1.846237	2.899001	1.767604	0.000000
6	C	2.626184	1.673892	1.641051	1.721967	1.709330
7	B	1.841945	2.945981	2.889937	3.381977	3.659399
8	B	2.788874	1.752876	3.422655	3.526152	2.922139
9	C	1.846515	2.729310	3.303682	2.883318	2.767385
10	B	2.905678	1.830838	3.664325	2.892075	1.736580
11	B	1.899830	2.838632	2.999941	1.740319	1.758570
12	Mn	2.420112	2.142198	1.929000	3.060950	3.290891
		6	7	8	9	10
6	C	0.000000				
7	B	3.325322	0.000000			
8	B	2.958496	1.736316	0.000000		
9	C	3.252453	1.645993	1.728160	0.000000	
10	B	2.796185	2.896589	1.777997	1.698461	0.000000
11	B	2.734222	2.948772	2.863172	1.674911	1.781244
12	Mn	2.140863	1.944043	2.154684	2.921677	3.262929
		11	12			
11	B	0.000000				
12	Mn	3.496870	0.000000			

Table 4. Energy ranking

	Initial structure	Final energy (a.u.)	D kcal/mole	Remarks
1	3-Anticuboh_Mn_v4_C2_m	-1651.06958759	0.00	
2	3-Anticuboh_Mn_v4_C2_j_r-178	-1651.06958620	0.00	
3	3-Anticuboh_Mn_v4_C2_k	-1651.06538765	2.64	
4	3-Anticuboh_Mn_v5_C2_k	-1651.06532786	2.67	
5	1-Icos_Mn_C2_f_r-86 i-23	-1651.06519599	2.76	
6	3-Anticuboh_Mn_v4_C2_q_r-356	-1651.06413135	3.42	
7	3-Anticuboh_Mn_v4_C2_b	-1651.06340365	3.88	
8	3-Anticuboh_Mn_v4_C2_d	-1651.06340312	3.88	
9	3-Anticuboh_Mn_v5_C2_z	-1651.06102929	5.37	
10	3-Anticuboh_Mn_v4_C2_l	-1651.06102918	5.37	
11	3-Anticuboh_Mn_v6_C2_r_r-35	-1651.06102918	5.37	
12	3-Anticuboh_Mn_v6_C2_r_r-159	-1651.06102916	5.37	
13	2-Cuboctaedru_Mn_v6_C2_g	-1651.06102886	5.37	
14	2-Cuboctaedru_Mn_v4_C2_d	-1651.06102875	5.37	
15	2-Cuboctaedru_Mn_v4_C2_q	-1651.06040132	5.76	
16	3-Anticuboh_Mn_v5_C2_u_r-26	-1651.06039980	5.77	
17	3-Anticuboh_Mn_v5_C2_u i-26	-1651.05973453	6.18	
18	3-Anticuboh_Mn_v5_C2_c	-1651.05958737	6.28	
19	2-Cuboctaedru_Mn_v4_C2_w	-1651.05958736	6.28	
20	2-Cuboctaedru_Mn_v6_C2_p	-1651.05958736	6.28	
21	3-Anticuboh_Mn_v6_C2_b	-1651.05958726	6.28	
22	3-Anticuboh_Mn_v5_C2_b_r-167	-1651.05821775	7.13	
23	3-Anticuboh_Mn_v6_C2_f_r-280	-1651.05821775	7.13	
24	3-Anticuboh_Mn_v5_C2_y	-1651.05821773	7.13	
25	3-Anticuboh_Mn_v6_C2_f_r-38	-1651.05821771	7.13	
26	3-Anticuboh_Mn_v6_C2_q	-1651.05821769	7.13	
27	2-Cuboctaedru_Mn_v6_C2_n	-1651.05821736	7.13	
28	2-Cuboctaedru_Mn_v4_C2_x	-1651.05821595	7.14	
29	2-Cuboctaedru_Mn_v6_C2_m	-1651.05664731	8.12	
30	3-Anticuboh_Mn_v6_C2_h	-1651.05664722	8.12	
31	2-Cuboctaedru_Mn_v4_C2_za	-1651.05664715	8.12	
32	3-Anticuboh_Mn_v5_C2_n	-1651.05664707	8.12	
33	3-Anticuboh_Mn_v5_C2_s	-1651.05664687	8.12	
34	3-Anticuboh_Mn_v4_C2_g_r-52	-1651.05572826	8.70	
35	3-Anticuboh_Mn_v4_C2_t_r-216	-1651.05572744	8.70	
36	3-Anticuboh_Mn_v4_C2_s	-1651.05572450	8.70	
37	3-Anticuboh_Mn_v5_C2_l	-1651.05564447	8.75	
38	2-Cuboctaedru_Mn_v4_C2_ze	-1651.05559529	8.78	

39	2-Cuboctaedru_Mn_v4_C2_n	-1651.05281312	10.53	
40	3-Anticuboh_Mn_v6_C2_n	-1651.05281307	10.53	
41	3-Anticuboh_Mn_v5_C2_x	-1651.05281302	10.53	
42	2-Cuboctaedru_Mn_v4_C2_p	-1651.05214350	10.95	
43	3-Anticuboh_Mn_v5_C2_p	-1651.05159518	11.29	
44	3-Anticuboh_Mn_v5_C2_e_r-39	-1651.04959634	12.54	
45	3-Anticuboh_Mn_v6_C2_e	-1651.04959630	12.54	
46	2-Cuboctaedru_Mn_v4_C2_y	-1651.04959614	12.54	
47	3-Anticuboh_Mn_v5_C2_j	-1651.04959596	12.54	
48	2-Cuboctaedru_Mn_v6_C2_o	-1651.04959559	12.54	
49	3-Anticuboh_Mn_v5_C2_e_i-39	-1651.04869234	13.11	
50	3-Anticuboh_Mn_v5_C2_o_r-28	-1651.04637070	14.57	
51	2-Cuboctaedru_Mn_v4_C2_r	-1651.04637006	14.57	
52	3-Anticuboh_Mn_v5_C2_o_i-28	-1651.04555509	15.08	
53	3-Anticuboh_Mn_v6_C2_i	-1651.04534955	15.21	
54	2-Cuboctaedru_Mn_v4_C2_s	-1651.04534255	15.21	
55	3-Anticuboh_Mn_v5_C2_t	-1651.04534218	15.21	
56	2-Cuboctaedru_Mn_v6_C2_e	-1651.04306852	16.64	
57	3-Anticuboh_Mn_v5_C2_v_r-183-34	-1651.04306840	16.64	
58	2-Cuboctaedru_Mn_v4_C2_f	-1651.04306794	16.64	
59	3-Anticuboh_Mn_v5_C2_v_r-183_i-34	-1651.04230568	17.12	
60	2-Cuboctaedru_Mn_v4_C2_o	-1651.04056125	18.21	
61	2-Cuboctaedru_Mn_v4_C2_b	-1651.04040030	18.32	
62	2-Cuboctaedru_Mn_v6_C2_c	-1651.04040028	18.32	
63	1-Icos_Mn_C2_e_r-31	-1651.03827020	19.65	C-C
64	3-Anticuboh_Mn_v4_C2_i	-1651.03827019	19.65	C-C
65	3-Anticuboh_Mn_v4_C2_h_r-33	-1651.03827017	19.65	C-C
66	3-Anticuboh_Mn_v4_C2_r	-1651.03827017	19.65	C-C
67	3-Anticuboh_Mn_v4_C2_h_r-255	-1651.03827014	19.65	C-C
68	3-Anticuboh_Mn_v4_C2_o	-1651.03827014	19.65	C-C
69	3-Anticuboh_Mn_v4_C2_e	-1651.03815317	19.73	C-C
70	2-Cuboctaedru_Mn_v6_C2_f	-1651.03580124	21.20	C-C
71	3-Anticuboh_Mn_v5_C2_d	-1651.03580121	21.20	C-C
72	2-Cuboctaedru_Mn_v6_C2_r	-1651.03580117	21.20	C-C
73	2-Cuboctaedru_Mn_v4_C2_v	-1651.03580107	21.20	C-C
74	3-Anticuboh_Mn_v6_C2_a	-1651.03580036	21.20	C-C
75	2-Cuboctaedru_Mn_v4_C2_zc	-1651.03570911	21.26	
76	3-Anticuboh_Mn_v6_C2_k_r-37	-1651.03570907	21.26	
77	3-Anticuboh_Mn_v6_C2_g_r-37	-1651.03490914	21.76	
78	3-Anticuboh_Mn_v4_C2_c	-1651.03490900	21.76	
79	2-Cuboctaedru_Mn_v6_C2_b	-1651.03490822	21.76	

80	3-Anticuboh_Mn_v6_C2_j	-1651.03414102	22.24	
81	3-Anticuboh_Mn_v6_C2_g i-37	-1651.03380688	22.45	
82	3-Anticuboh_Mn_v5_C2_h	-1651.03175820	23.74	C-C
83	3-Anticuboh_Mn_v4_C2_f	-1651.03174863	23.74	C-C
84	3-Anticuboh_Mn_v5_C2_w	-1651.02789812	26.16	C-C
85	3-Anticuboh_Mn_v5_C2_a_r-115	-1651.02789797	26.16	C-C
86	3-Anticuboh_Mn_v5_C2_a_r-255	-1651.02789788	26.16	C-C
87	2-Cuboctaedru_Mn_v4_C2_z	-1651.02789776	26.16	C-C
88	3-Anticuboh_Mn_v5_C2_q_r-26	-1651.02481497	28.09	C-C
89	2-Cuboctaedru_Mn_v4_C2_c	-1651.02480990	28.10	C-C
90	3-Anticuboh_Mn_v5_C2_q i-26	-1651.02403733	28.58	C-C
91	2-Cuboctaedru_Mn_v4_C2_e	-1651.02374585	28.77	C-C
92	2-Cuboctaedru_Mn_v6_C2_d	-1651.02374583	28.77	C-C
93	3-Anticuboh_Mn_v5_C2_i	-1651.02282600	29.34	
94	3-Anticuboh_Mn_v6_C2_s	-1651.02228637	29.68	
95	2-Cuboctaedru_Mn_v6_C2_q	-1651.02227742	29.69	
96	3-Anticuboh_Mn_v4_C2_n	-1651.02226980	29.69	
97	3-Anticuboh_Mn_v6_C2_c	-1651.02226707	29.69	
98	2-Cuboctaedru_Mn_v4_C2_a	-1651.02180691	29.98	
99	2-Cuboctaedru_Mn_v6_C2_h	-1651.02180646	29.98	
100	1-Icos_Mn_C2_g	-1651.02160615	30.11	
101	2-Cuboctaedru_Mn_v4_C2_u	-1651.02123382	30.34	C-C
102	2-Cuboctaedru_Mn_v6_C2_l	-1651.02123372	30.34	C-C
103	3-Anticuboh_Mn_v5_C2_r	-1651.02123362	30.34	C-C
104	3-Anticuboh_Mn_v5_C2_v_r-79	-1651.02025137	30.96	
105	2-Cuboctaedru_Mn_v4_C2_i	-1651.01986195	31.20	C-C
106	3-Anticuboh_Mn_v6_C2_t	-1651.01986178	31.20	C-C
107	1-Icos_Mn_C2_f_r-86-23	-1651.01801312	32.36	
108	2-Cuboctaedru_Mn_v4_C2_h	-1651.01728792	32.82	
109	2-Cuboctaedru_Mn_v4_C2_j	-1651.01691749	33.05	
110	1-Icos_Mn_C2_d	-1651.01691746	33.05	
111	2-Cuboctaedru_Mn_v4_C2_g	-1651.01644068	33.35	
112	1-Icos_Mn_C2_i	-1651.01590794	33.68	
113	1-Icos_Mn_C2_f i-86	-1651.01555611	33.90	
114	1-Icos_Mn_C2_b	-1651.01467198	34.46	
115	2-Cuboctaedru_Mn_v6_C2_k	-1651.01372420	35.05	C-C
116	2-Cuboctaedru_Mn_v4_C2_t	-1651.01284632	35.61	
117	3-Anticuboh_Mn_v5_C2_f	-1651.01284600	35.61	
118	2-Cuboctaedru_Mn_v6_C2_i	-1651.01181034	36.26	C-C
119	2-Cuboctaedru_Mn_v4_C2_zd	-1651.01180813	36.26	C-C
120	2-Cuboctaedru_Mn_v6_C2_a	-1651.01103579	36.74	C-C

121	3-Anticuboh_Mn_v6_C2_l_r-21	-1651.01103525	36.74	C-C
122	2-Cuboctaedru_Mn_v4_C2_m	-1651.01102934	36.75	C-C
123	3-Anticuboh_Mn_v6_C2_m_r-23	-1651.00787593	38.72	C-C
124	3-Anticuboh_Mn_v6_C2_m_r-36	-1651.00787583	38.72	C-C
125	2-Cuboctaedru_Mn_v4_C2_l	-1651.00787545	38.72	C-C
126	3-Anticuboh_Mn_v4_C2_a_r-195	-1651.00787536	38.72	C-C
127	3-Anticuboh_Mn_v4_C2_p	-1651.00472989	40.70	
128	3-Anticuboh_Mn_v6_C2_r_imag	-1650.99966486	43.88	
129	3-Anticuboh_Mn_v6_C2_p_r-26-93	-1650.99637982	45.94	
130	2-Cuboctaedru_Mn_v6_C2_j	-1650.99637975	45.94	
131	3-Anticuboh_Mn_v6_C2_p_r-91	-1650.99637829	45.94	
132	1-Icos_Mn_C2_e_i-31	-1650.99133797	49.10	C-C
133	1-Icos_Mn_C2_h_r-44	-1650.99132418	49.11	C-C
134	1-Icos_Mn_C2_h_i-44	-1650.99130329	49.12	C-C
135	1-Icos_Mn_C2_c_r-57	-1650.99077020	49.46	C-C
136	2-Cuboctaedru_Mn_v4_C2_zb	-1650.99076615	49.46	C-C
137	1-Icos_Mn_C2_c_i-97	-1650.99057774	49.58	C-C
138	2-Cuboctaedru_Mn_v4_C2_k	-1650.99040876	49.68	C-C
139	1-Icos_Mn_C2_a	-1650.98869319	50.76	C-C
140	3-Anticuboh_Mn_v6_C2_p_r-26_i-93	-1650.98130720	55.40	
141	3-Anticuboh_Mn_v6_C2_p_imag	-1650.98128349	55.41	
142	3-Anticuboh_Mn_v4_C2_t_r-64	-1650.97931575	56.65	
143	3-Anticuboh_Mn_v5_C2_zc	-1650.97884934	56.94	
144	3-Anticuboh_Mn_v6_C2_f_imag	-1650.97870036	57.03	
145	3-Anticuboh_Mn_v6_C2_m_imag	-1650.97663164	58.33	C-C
146	3-Anticuboh_Mn_v6_C2_o	-1650.97638073	58.49	C-C
147	3-Anticuboh_Mn_v6_C2_k_i-37	-1650.97543698	59.08	
148	3-Anticuboh_Mn_v6_C2_l_r-27	-1650.97401180	59.97	C-C
149	3-Anticuboh_Mn_v6_C2_l_r-284	-1650.97401043	59.97	C-C
150	3-Anticuboh_Mn_v5_C2_b_i-167	-1650.96523182	65.48	
151	3-Anticuboh_Mn_v6_C2_d_r-49	-1650.96194770	67.54	C-C
152	3-Anticuboh_Mn_v5_C2_v_imag	-1650.96144637	67.86	
153	3-Anticuboh_Mn_v6_C2_d	-1650.96039328	68.52	C-C
154	3-Anticuboh_Mn_v4_C2_g_i-52	-1650.95951327	69.07	
155	3-Anticuboh_Mn_v6_C2_l_imag	-1650.95703947	70.62	C-C
156	3-Anticuboh_Mn_v5_C2_g	-1650.95574536	71.44	
157	3-Anticuboh_Mn_v5_C2_a_imag	-1650.95338856	72.91	C-C
158	3-Anticuboh_Mn_v5_C2_m	-1650.93830897	82.38	C-C
159	3-Anticuboh_Mn_v5_C2_za	-1650.92734428	89.26	C-C
160	3-Anticuboh_Mn_v4_C2_a_i-195	-1650.92327084	91.81	C-C
161	3-Anticuboh_Mn_v4_C2_t_imag	-1650.91814696	95.03	

162	3-Anticuboh_Mn_v4_C2_q i-356	-1650.91484404	97.10	C-C
163	3-Anticuboh_Mn_v5_C2_zd	-1650.91184754	98.98	C-C
164	3-Anticuboh_Mn_v4_C2_j i-178	-1650.90305151	104.50	
165	3-Anticuboh_Mn_v4_C2_h imag	-1650.87928681	119.41	

12-vertex $\text{CpReC}_2\text{B}_9\text{H}_{11}$

Table 1. Initial structures (one example from each family) 128 structures in total

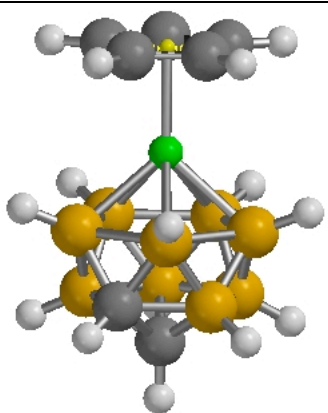
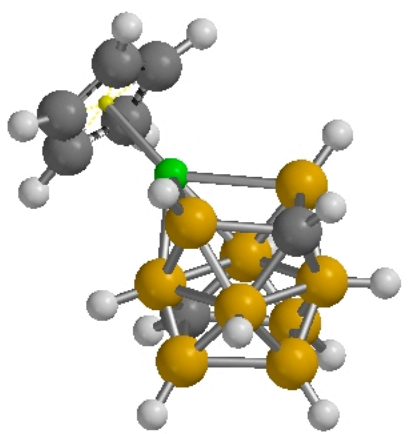
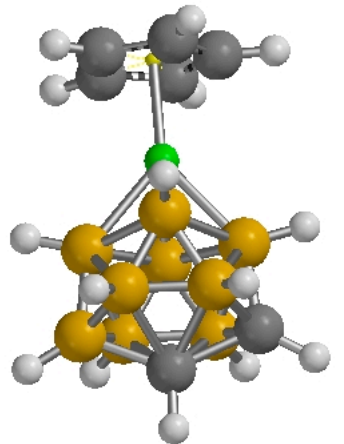
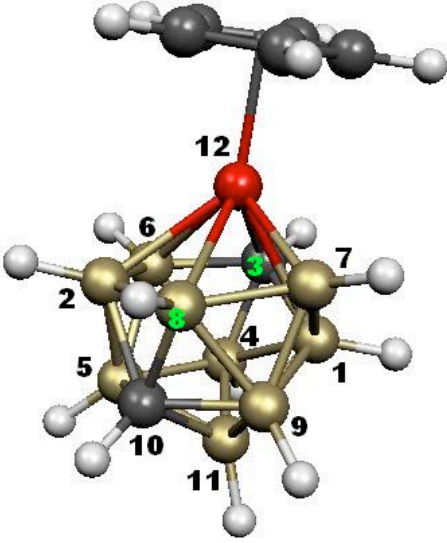
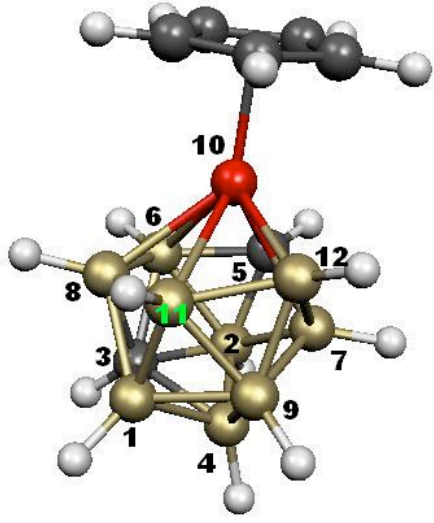
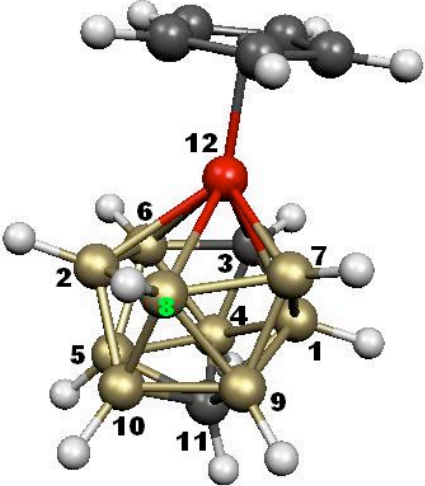
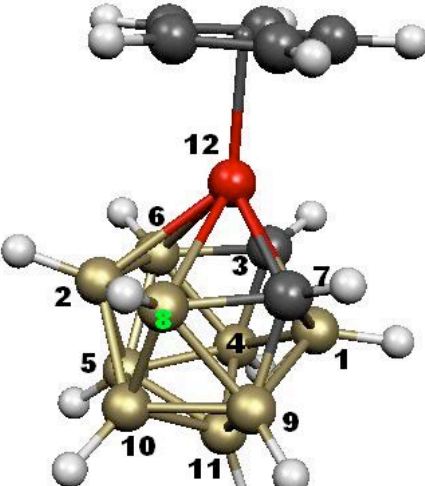
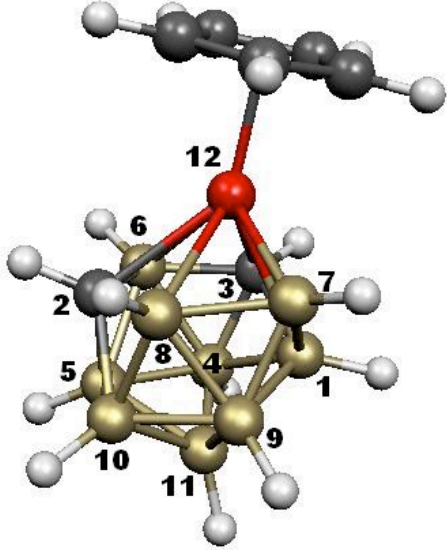
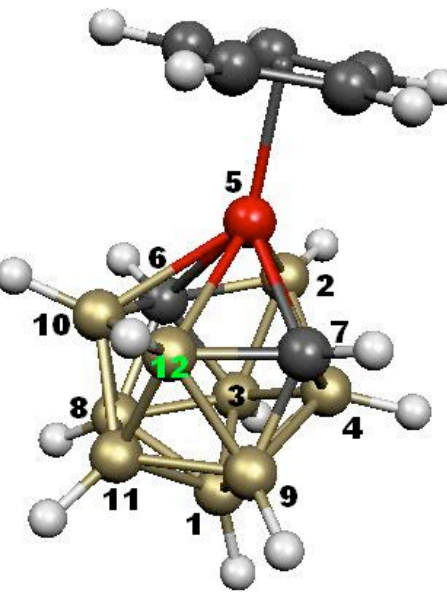
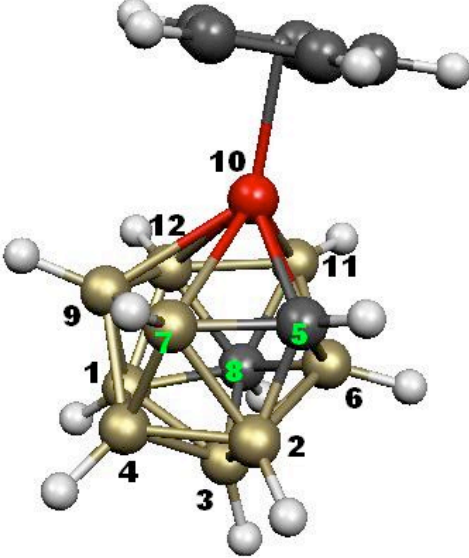
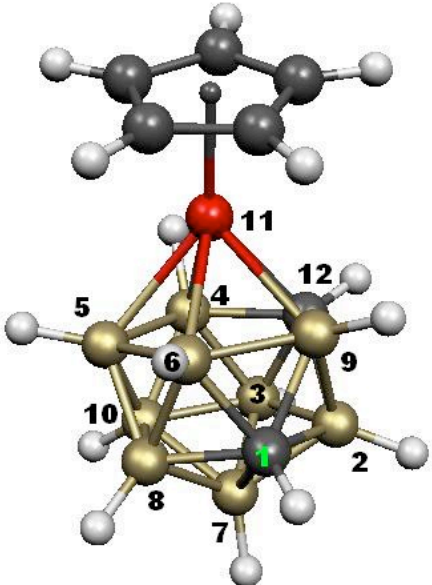
Initial structures
 <p>1. Icosahedron 9 structures</p>
 <p>2. Cubeoctahedron 49 structures</p>
 <p>3. Anticubeoctahedron 70 structures</p>

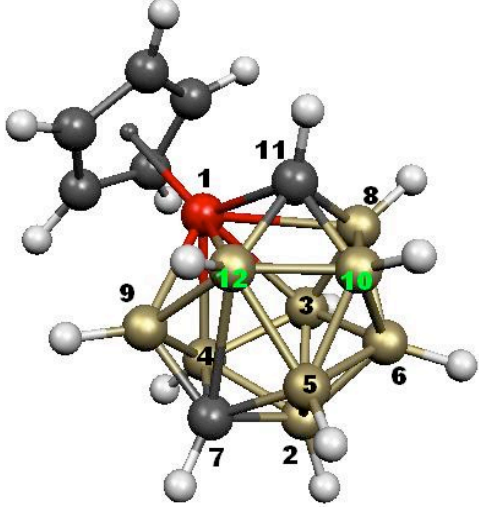
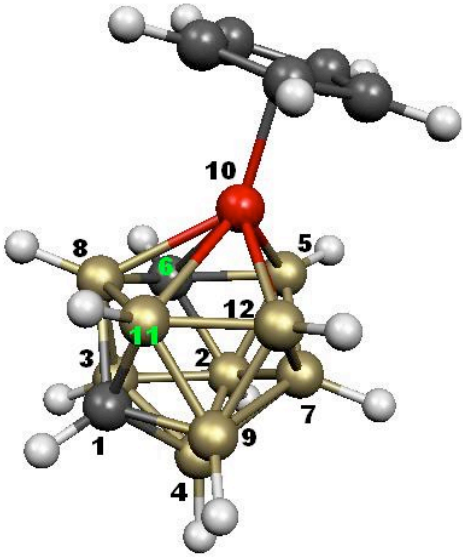
Table 3. Distance table for the best structures

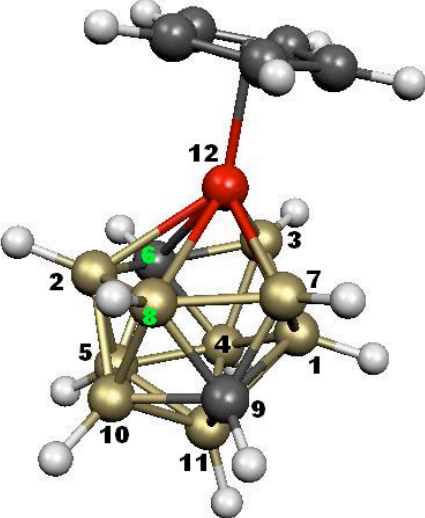
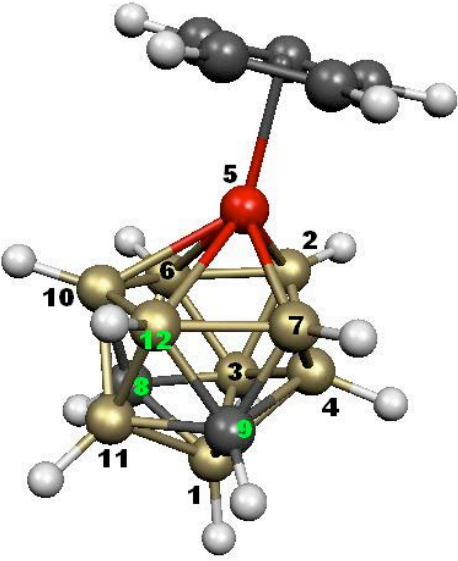
 <p>1. -578.49560700 0.</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.107156</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>1.715316</td><td>2.856152</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.945711</td><td>2.910575</td><td>1.609168</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.878882</td><td>1.841128</td><td>2.755980</td><td>1.778903</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.774752</td><td>1.784511</td><td>1.660472</td><td>1.831845</td><td>1.789473</td></tr> <tr><td>7 B</td><td>1.998689</td><td>3.025658</td><td>3.014076</td><td>3.637849</td><td>3.781355</td></tr> <tr><td>8 B</td><td>2.811595</td><td>1.778100</td><td>3.414170</td><td>3.630281</td><td>2.926446</td></tr> <tr><td>9 B</td><td>1.935433</td><td>2.867710</td><td>3.308575</td><td>3.082097</td><td>2.897028</td></tr> <tr><td>10 C</td><td>2.747841</td><td>1.776830</td><td>3.377436</td><td>2.797001</td><td>1.658119</td></tr> <tr><td>11 B</td><td>1.882900</td><td>2.850205</td><td>2.793646</td><td>1.757134</td><td>1.773757</td></tr> <tr><td>12 Re</td><td>2.465549</td><td>2.253088</td><td>2.028091</td><td>3.215525</td><td>3.390264</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>3.623427</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.151572</td><td>1.754311</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.578904</td><td>1.741225</td><td>1.791820</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>2.825424</td><td>2.851054</td><td>1.713171</td><td>1.690393</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.870880</td><td>3.066903</td><td>2.868716</td><td>1.758153</td><td>1.680725</td></tr> <tr><td>12 Re</td><td>2.314537</td><td>2.062211</td><td>2.300844</td><td>3.127543</td><td>3.252357</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Re</td><td>3.582023</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	3.107156	0.000000				3 C	1.715316	2.856152	0.000000			4 B	1.945711	2.910575	1.609168	0.000000		5 B	2.878882	1.841128	2.755980	1.778903	0.000000	6 B	2.774752	1.784511	1.660472	1.831845	1.789473	7 B	1.998689	3.025658	3.014076	3.637849	3.781355	8 B	2.811595	1.778100	3.414170	3.630281	2.926446	9 B	1.935433	2.867710	3.308575	3.082097	2.897028	10 C	2.747841	1.776830	3.377436	2.797001	1.658119	11 B	1.882900	2.850205	2.793646	1.757134	1.773757	12 Re	2.465549	2.253088	2.028091	3.215525	3.390264		6	7	8	9	10	6 B	0.000000					7 B	3.623427	0.000000				8 B	3.151572	1.754311	0.000000			9 B	3.578904	1.741225	1.791820	0.000000		10 C	2.825424	2.851054	1.713171	1.690393	0.000000	11 B	2.870880	3.066903	2.868716	1.758153	1.680725	12 Re	2.314537	2.062211	2.300844	3.127543	3.252357		11	12				11 B	0.000000					12 Re	3.582023	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	3.107156	0.000000																																																																																																																																															
3 C	1.715316	2.856152	0.000000																																																																																																																																														
4 B	1.945711	2.910575	1.609168	0.000000																																																																																																																																													
5 B	2.878882	1.841128	2.755980	1.778903	0.000000																																																																																																																																												
6 B	2.774752	1.784511	1.660472	1.831845	1.789473																																																																																																																																												
7 B	1.998689	3.025658	3.014076	3.637849	3.781355																																																																																																																																												
8 B	2.811595	1.778100	3.414170	3.630281	2.926446																																																																																																																																												
9 B	1.935433	2.867710	3.308575	3.082097	2.897028																																																																																																																																												
10 C	2.747841	1.776830	3.377436	2.797001	1.658119																																																																																																																																												
11 B	1.882900	2.850205	2.793646	1.757134	1.773757																																																																																																																																												
12 Re	2.465549	2.253088	2.028091	3.215525	3.390264																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	3.623427	0.000000																																																																																																																																															
8 B	3.151572	1.754311	0.000000																																																																																																																																														
9 B	3.578904	1.741225	1.791820	0.000000																																																																																																																																													
10 C	2.825424	2.851054	1.713171	1.690393	0.000000																																																																																																																																												
11 B	2.870880	3.066903	2.868716	1.758153	1.680725																																																																																																																																												
12 Re	2.314537	2.062211	2.300844	3.127543	3.252357																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 Re	3.582023	0.000000																																																																																																																																															
 <p>2. -578.49406073 +1.0</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>2.905679</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>1.662567</td><td>1.685473</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.764875</td><td>1.762589</td><td>1.698792</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>3.522406</td><td>1.605316</td><td>2.634380</td><td>2.786955</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.925748</td><td>1.823881</td><td>1.722283</td><td>2.867278</td><td>1.648515</td></tr> <tr><td>7 B</td><td>2.897083</td><td>1.932563</td><td>2.732114</td><td>1.870653</td><td>1.693971</td></tr> <tr><td>8 B</td><td>1.835569</td><td>2.919211</td><td>1.784934</td><td>2.853217</td><td>2.881625</td></tr> <tr><td>9 B</td><td>1.778329</td><td>3.072302</td><td>2.778703</td><td>1.740225</td><td>3.293285</td></tr> <tr><td>10 Re</td><td>3.379403</td><td>3.216283</td><td>3.258892</td><td>3.574500</td><td>2.042564</td></tr> <tr><td>11 B</td><td>1.770789</td><td>3.647160</td><td>2.829002</td><td>2.868402</td><td>3.451159</td></tr> <tr><td>12 B</td><td>2.980839</td><td>3.681374</td><td>3.667158</td><td>3.095570</td><td>3.050281</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.743458</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.797095</td><td>3.117453</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.549186</td><td>1.939652</td><td>2.853866</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>2.286066</td><td>2.473088</td><td>2.255776</td><td>3.112390</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.151958</td><td>2.855553</td><td>1.768199</td><td>1.795227</td><td>2.330216</td></tr> <tr><td>12 B</td><td>3.614581</td><td>2.073160</td><td>3.018504</td><td>1.762522</td><td>2.054819</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.764797</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.905679	0.000000				3 C	1.662567	1.685473	0.000000			4 B	1.764875	1.762589	1.698792	0.000000		5 C	3.522406	1.605316	2.634380	2.786955	0.000000	6 B	2.925748	1.823881	1.722283	2.867278	1.648515	7 B	2.897083	1.932563	2.732114	1.870653	1.693971	8 B	1.835569	2.919211	1.784934	2.853217	2.881625	9 B	1.778329	3.072302	2.778703	1.740225	3.293285	10 Re	3.379403	3.216283	3.258892	3.574500	2.042564	11 B	1.770789	3.647160	2.829002	2.868402	3.451159	12 B	2.980839	3.681374	3.667158	3.095570	3.050281		6	7	8	9	10	6 B	0.000000					7 B	2.743458	0.000000				8 B	1.797095	3.117453	0.000000			9 B	3.549186	1.939652	2.853866	0.000000		10 Re	2.286066	2.473088	2.255776	3.112390	0.000000	11 B	3.151958	2.855553	1.768199	1.795227	2.330216	12 B	3.614581	2.073160	3.018504	1.762522	2.054819		11	12				11 B	0.000000					12 B	1.764797	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	2.905679	0.000000																																																																																																																																															
3 C	1.662567	1.685473	0.000000																																																																																																																																														
4 B	1.764875	1.762589	1.698792	0.000000																																																																																																																																													
5 C	3.522406	1.605316	2.634380	2.786955	0.000000																																																																																																																																												
6 B	2.925748	1.823881	1.722283	2.867278	1.648515																																																																																																																																												
7 B	2.897083	1.932563	2.732114	1.870653	1.693971																																																																																																																																												
8 B	1.835569	2.919211	1.784934	2.853217	2.881625																																																																																																																																												
9 B	1.778329	3.072302	2.778703	1.740225	3.293285																																																																																																																																												
10 Re	3.379403	3.216283	3.258892	3.574500	2.042564																																																																																																																																												
11 B	1.770789	3.647160	2.829002	2.868402	3.451159																																																																																																																																												
12 B	2.980839	3.681374	3.667158	3.095570	3.050281																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	2.743458	0.000000																																																																																																																																															
8 B	1.797095	3.117453	0.000000																																																																																																																																														
9 B	3.549186	1.939652	2.853866	0.000000																																																																																																																																													
10 Re	2.286066	2.473088	2.255776	3.112390	0.000000																																																																																																																																												
11 B	3.151958	2.855553	1.768199	1.795227	2.330216																																																																																																																																												
12 B	3.614581	2.073160	3.018504	1.762522	2.054819																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.764797	0.000000																																																																																																																																															

 <p>3. -578.49027654 +3.3</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>3.095795</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>1.694124</td><td>2.899394</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.939218</td><td>2.907724</td><td>1.603347</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.879598</td><td>1.832312</td><td>2.769339</td><td>1.773141</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.747086</td><td>1.810129</td><td>1.668726</td><td>1.818570</td><td>1.786934</td></tr> <tr><td>7 B</td><td>1.974171</td><td>3.047443</td><td>3.022297</td><td>3.627037</td><td>3.796076</td></tr> <tr><td>8 B</td><td>2.802352</td><td>1.791005</td><td>3.451239</td><td>3.631620</td><td>2.943147</td></tr> <tr><td>9 B</td><td>1.938555</td><td>2.866641</td><td>3.320020</td><td>3.070931</td><td>2.907153</td></tr> <tr><td>10 B</td><td>2.894707</td><td>1.826147</td><td>3.546525</td><td>2.914220</td><td>1.731229</td></tr> <tr><td>11 C</td><td>1.803492</td><td>2.693693</td><td>2.680222</td><td>1.691248</td><td>1.699619</td></tr> <tr><td>12 Re</td><td>2.414358</td><td>2.278896</td><td>2.034454</td><td>3.193210</td><td>3.384210</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>3.626193</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.173709</td><td>1.774099</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.579846</td><td>1.751709</td><td>1.791850</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.945151</td><td>2.980026</td><td>1.776119</td><td>1.780299</td><td>0.000000</td></tr> <tr><td>11 C</td><td>2.733612</td><td>2.949424</td><td>2.735245</td><td>1.686743</td><td>1.692533</td></tr> <tr><td>12 Re</td><td>2.309025</td><td>2.054793</td><td>2.317265</td><td>3.119991</td><td>3.379024</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Re</td><td>3.407283</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	3.095795	0.000000				3 C	1.694124	2.899394	0.000000			4 B	1.939218	2.907724	1.603347	0.000000		5 B	2.879598	1.832312	2.769339	1.773141	0.000000	6 B	2.747086	1.810129	1.668726	1.818570	1.786934	7 B	1.974171	3.047443	3.022297	3.627037	3.796076	8 B	2.802352	1.791005	3.451239	3.631620	2.943147	9 B	1.938555	2.866641	3.320020	3.070931	2.907153	10 B	2.894707	1.826147	3.546525	2.914220	1.731229	11 C	1.803492	2.693693	2.680222	1.691248	1.699619	12 Re	2.414358	2.278896	2.034454	3.193210	3.384210		6	7	8	9	10	6 B	0.000000					7 B	3.626193	0.000000				8 B	3.173709	1.774099	0.000000			9 B	3.579846	1.751709	1.791850	0.000000		10 B	2.945151	2.980026	1.776119	1.780299	0.000000	11 C	2.733612	2.949424	2.735245	1.686743	1.692533	12 Re	2.309025	2.054793	2.317265	3.119991	3.379024		11	12				11 C	0.000000					12 Re	3.407283	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	3.095795	0.000000																																																																																																																																															
3 C	1.694124	2.899394	0.000000																																																																																																																																														
4 B	1.939218	2.907724	1.603347	0.000000																																																																																																																																													
5 B	2.879598	1.832312	2.769339	1.773141	0.000000																																																																																																																																												
6 B	2.747086	1.810129	1.668726	1.818570	1.786934																																																																																																																																												
7 B	1.974171	3.047443	3.022297	3.627037	3.796076																																																																																																																																												
8 B	2.802352	1.791005	3.451239	3.631620	2.943147																																																																																																																																												
9 B	1.938555	2.866641	3.320020	3.070931	2.907153																																																																																																																																												
10 B	2.894707	1.826147	3.546525	2.914220	1.731229																																																																																																																																												
11 C	1.803492	2.693693	2.680222	1.691248	1.699619																																																																																																																																												
12 Re	2.414358	2.278896	2.034454	3.193210	3.384210																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	3.626193	0.000000																																																																																																																																															
8 B	3.173709	1.774099	0.000000																																																																																																																																														
9 B	3.579846	1.751709	1.791850	0.000000																																																																																																																																													
10 B	2.945151	2.980026	1.776119	1.780299	0.000000																																																																																																																																												
11 C	2.733612	2.949424	2.735245	1.686743	1.692533																																																																																																																																												
12 Re	2.309025	2.054793	2.317265	3.119991	3.379024																																																																																																																																												
	11	12																																																																																																																																															
11 C	0.000000																																																																																																																																																
12 Re	3.407283	0.000000																																																																																																																																															
 <p>4. -578.48957885 +3.8 Cs</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>3.116049</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>1.764183</td><td>2.878498</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.957884</td><td>2.899639</td><td>1.607092</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.916330</td><td>1.828235</td><td>2.778163</td><td>1.790021</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.799950</td><td>1.780760</td><td>1.661244</td><td>1.848571</td><td>1.802057</td></tr> <tr><td>7 C</td><td>1.764183</td><td>2.878498</td><td>2.869600</td><td>3.383417</td><td>3.565853</td></tr> <tr><td>8 B</td><td>2.799950</td><td>1.780760</td><td>3.430951</td><td>3.621952</td><td>2.952305</td></tr> <tr><td>9 B</td><td>1.957884</td><td>2.899639</td><td>3.383417</td><td>3.089200</td><td>2.929797</td></tr> <tr><td>10 B</td><td>2.916330</td><td>1.828235</td><td>3.565853</td><td>2.929797</td><td>1.741400</td></tr> <tr><td>11 B</td><td>1.949991</td><td>2.822816</td><td>2.851601</td><td>1.768402</td><td>1.757922</td></tr> <tr><td>12 Re</td><td>2.436817</td><td>2.297249</td><td>2.012709</td><td>3.185966</td><td>3.406019</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 C</td><td>3.430951</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.140400</td><td>1.661244</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.621952</td><td>1.607092</td><td>1.848571</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.952305</td><td>2.778163</td><td>1.802057</td><td>1.790021</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.884986</td><td>2.851601</td><td>2.884986</td><td>1.768402</td><td>1.757922</td></tr> <tr><td>12 Re</td><td>2.300723</td><td>2.012709</td><td>2.300723</td><td>3.185966</td><td>3.406019</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Re</td><td>3.599733</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	3.116049	0.000000				3 C	1.764183	2.878498	0.000000			4 B	1.957884	2.899639	1.607092	0.000000		5 B	2.916330	1.828235	2.778163	1.790021	0.000000	6 B	2.799950	1.780760	1.661244	1.848571	1.802057	7 C	1.764183	2.878498	2.869600	3.383417	3.565853	8 B	2.799950	1.780760	3.430951	3.621952	2.952305	9 B	1.957884	2.899639	3.383417	3.089200	2.929797	10 B	2.916330	1.828235	3.565853	2.929797	1.741400	11 B	1.949991	2.822816	2.851601	1.768402	1.757922	12 Re	2.436817	2.297249	2.012709	3.185966	3.406019		6	7	8	9	10	6 B	0.000000					7 C	3.430951	0.000000				8 B	3.140400	1.661244	0.000000			9 B	3.621952	1.607092	1.848571	0.000000		10 B	2.952305	2.778163	1.802057	1.790021	0.000000	11 B	2.884986	2.851601	2.884986	1.768402	1.757922	12 Re	2.300723	2.012709	2.300723	3.185966	3.406019		11	12				11 B	0.000000					12 Re	3.599733	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	3.116049	0.000000																																																																																																																																															
3 C	1.764183	2.878498	0.000000																																																																																																																																														
4 B	1.957884	2.899639	1.607092	0.000000																																																																																																																																													
5 B	2.916330	1.828235	2.778163	1.790021	0.000000																																																																																																																																												
6 B	2.799950	1.780760	1.661244	1.848571	1.802057																																																																																																																																												
7 C	1.764183	2.878498	2.869600	3.383417	3.565853																																																																																																																																												
8 B	2.799950	1.780760	3.430951	3.621952	2.952305																																																																																																																																												
9 B	1.957884	2.899639	3.383417	3.089200	2.929797																																																																																																																																												
10 B	2.916330	1.828235	3.565853	2.929797	1.741400																																																																																																																																												
11 B	1.949991	2.822816	2.851601	1.768402	1.757922																																																																																																																																												
12 Re	2.436817	2.297249	2.012709	3.185966	3.406019																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 C	3.430951	0.000000																																																																																																																																															
8 B	3.140400	1.661244	0.000000																																																																																																																																														
9 B	3.621952	1.607092	1.848571	0.000000																																																																																																																																													
10 B	2.952305	2.778163	1.802057	1.790021	0.000000																																																																																																																																												
11 B	2.884986	2.851601	2.884986	1.768402	1.757922																																																																																																																																												
12 Re	2.300723	2.012709	2.300723	3.185966	3.406019																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 Re	3.599733	0.000000																																																																																																																																															

 <p>5. -578.48906733 +4.1</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 C</td><td>2.962157</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>1.699403</td><td>2.761144</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.949009</td><td>2.767152</td><td>1.607611</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.873224</td><td>1.743004</td><td>2.762267</td><td>1.763287</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.747520</td><td>1.703610</td><td>1.657853</td><td>1.825774</td><td>1.801323</td></tr> <tr><td>7 B</td><td>2.038848</td><td>2.936662</td><td>3.017429</td><td>3.669345</td><td>3.807797</td></tr> <tr><td>8 B</td><td>2.828024</td><td>1.682146</td><td>3.395434</td><td>3.620761</td><td>2.918575</td></tr> <tr><td>9 B</td><td>1.931105</td><td>2.710573</td><td>3.285579</td><td>3.086621</td><td>2.892991</td></tr> <tr><td>10 B</td><td>2.889561</td><td>1.750503</td><td>3.529428</td><td>2.917617</td><td>1.729268</td></tr> <tr><td>11 B</td><td>1.892303</td><td>2.688802</td><td>2.805640</td><td>1.784125</td><td>1.766796</td></tr> <tr><td>12 Re</td><td>2.481302</td><td>2.260992</td><td>2.036193</td><td>3.233129</td><td>3.432715</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>3.589944</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.077589</td><td>1.777595</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.532231</td><td>1.752701</td><td>1.807139</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.929498</td><td>2.987468</td><td>1.792732</td><td>1.761397</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.871229</td><td>3.104435</td><td>2.876802</td><td>1.760438</td><td>1.747275</td></tr> <tr><td>12 Re</td><td>2.297519</td><td>2.050886</td><td>2.299830</td><td>3.122503</td><td>3.427975</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Re</td><td>3.616693</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	2.962157	0.000000				3 C	1.699403	2.761144	0.000000			4 B	1.949009	2.767152	1.607611	0.000000		5 B	2.873224	1.743004	2.762267	1.763287	0.000000	6 B	2.747520	1.703610	1.657853	1.825774	1.801323	7 B	2.038848	2.936662	3.017429	3.669345	3.807797	8 B	2.828024	1.682146	3.395434	3.620761	2.918575	9 B	1.931105	2.710573	3.285579	3.086621	2.892991	10 B	2.889561	1.750503	3.529428	2.917617	1.729268	11 B	1.892303	2.688802	2.805640	1.784125	1.766796	12 Re	2.481302	2.260992	2.036193	3.233129	3.432715		6	7	8	9	10	6 B	0.000000					7 B	3.589944	0.000000				8 B	3.077589	1.777595	0.000000			9 B	3.532231	1.752701	1.807139	0.000000		10 B	2.929498	2.987468	1.792732	1.761397	0.000000	11 B	2.871229	3.104435	2.876802	1.760438	1.747275	12 Re	2.297519	2.050886	2.299830	3.122503	3.427975		11	12				11 B	0.000000					12 Re	3.616693	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 C	2.962157	0.000000																																																																																																																																															
3 C	1.699403	2.761144	0.000000																																																																																																																																														
4 B	1.949009	2.767152	1.607611	0.000000																																																																																																																																													
5 B	2.873224	1.743004	2.762267	1.763287	0.000000																																																																																																																																												
6 B	2.747520	1.703610	1.657853	1.825774	1.801323																																																																																																																																												
7 B	2.038848	2.936662	3.017429	3.669345	3.807797																																																																																																																																												
8 B	2.828024	1.682146	3.395434	3.620761	2.918575																																																																																																																																												
9 B	1.931105	2.710573	3.285579	3.086621	2.892991																																																																																																																																												
10 B	2.889561	1.750503	3.529428	2.917617	1.729268																																																																																																																																												
11 B	1.892303	2.688802	2.805640	1.784125	1.766796																																																																																																																																												
12 Re	2.481302	2.260992	2.036193	3.233129	3.432715																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	3.589944	0.000000																																																																																																																																															
8 B	3.077589	1.777595	0.000000																																																																																																																																														
9 B	3.532231	1.752701	1.807139	0.000000																																																																																																																																													
10 B	2.929498	2.987468	1.792732	1.761397	0.000000																																																																																																																																												
11 B	2.871229	3.104435	2.876802	1.760438	1.747275																																																																																																																																												
12 Re	2.297519	2.050886	2.299830	3.122503	3.427975																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 Re	3.616693	0.000000																																																																																																																																															
 <p>6. -578.48854849 +4.4</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>3.103940</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.729952</td><td>1.770803</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.919767</td><td>2.015483</td><td>1.899188</td><td>0.000000</td><td></td></tr> <tr><td>5 Re</td><td>3.608771</td><td>2.035028</td><td>3.125576</td><td>2.468937</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.740829</td><td>1.683654</td><td>1.703686</td><td>2.685678</td><td>2.268665</td></tr> <tr><td>7 C</td><td>2.792872</td><td>3.003823</td><td>3.256134</td><td>1.703539</td><td>2.032836</td></tr> <tr><td>8 B</td><td>1.760051</td><td>2.973474</td><td>1.765881</td><td>2.912550</td><td>3.423034</td></tr> <tr><td>9 B</td><td>1.771746</td><td>3.664152</td><td>3.052087</td><td>1.989373</td><td>3.228138</td></tr> <tr><td>10 B</td><td>2.840047</td><td>2.979180</td><td>2.828537</td><td>3.114004</td><td>2.277943</td></tr> <tr><td>11 B</td><td>1.781732</td><td>3.787131</td><td>2.878161</td><td>2.912765</td><td>3.409200</td></tr> <tr><td>12 B</td><td>2.870340</td><td>3.585848</td><td>3.531564</td><td>2.773883</td><td>2.299700</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 C</td><td>3.290009</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.708569</td><td>3.532888</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.494412</td><td>1.609999</td><td>2.921729</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.690108</td><td>2.876421</td><td>1.842829</td><td>2.911225</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.815063</td><td>2.763426</td><td>1.730431</td><td>1.773759</td><td>1.840249</td></tr> <tr><td>12 B</td><td>3.030849</td><td>1.659005</td><td>2.950061</td><td>1.817229</td><td>1.803721</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.794371</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	3.103940	0.000000				3 B	1.729952	1.770803	0.000000			4 B	1.919767	2.015483	1.899188	0.000000		5 Re	3.608771	2.035028	3.125576	2.468937	0.000000	6 C	2.740829	1.683654	1.703686	2.685678	2.268665	7 C	2.792872	3.003823	3.256134	1.703539	2.032836	8 B	1.760051	2.973474	1.765881	2.912550	3.423034	9 B	1.771746	3.664152	3.052087	1.989373	3.228138	10 B	2.840047	2.979180	2.828537	3.114004	2.277943	11 B	1.781732	3.787131	2.878161	2.912765	3.409200	12 B	2.870340	3.585848	3.531564	2.773883	2.299700		6	7	8	9	10	6 C	0.000000					7 C	3.290009	0.000000				8 B	1.708569	3.532888	0.000000			9 B	3.494412	1.609999	2.921729	0.000000		10 B	1.690108	2.876421	1.842829	2.911225	0.000000	11 B	2.815063	2.763426	1.730431	1.773759	1.840249	12 B	3.030849	1.659005	2.950061	1.817229	1.803721		11	12				11 B	0.000000					12 B	1.794371	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	3.103940	0.000000																																																																																																																																															
3 B	1.729952	1.770803	0.000000																																																																																																																																														
4 B	1.919767	2.015483	1.899188	0.000000																																																																																																																																													
5 Re	3.608771	2.035028	3.125576	2.468937	0.000000																																																																																																																																												
6 C	2.740829	1.683654	1.703686	2.685678	2.268665																																																																																																																																												
7 C	2.792872	3.003823	3.256134	1.703539	2.032836																																																																																																																																												
8 B	1.760051	2.973474	1.765881	2.912550	3.423034																																																																																																																																												
9 B	1.771746	3.664152	3.052087	1.989373	3.228138																																																																																																																																												
10 B	2.840047	2.979180	2.828537	3.114004	2.277943																																																																																																																																												
11 B	1.781732	3.787131	2.878161	2.912765	3.409200																																																																																																																																												
12 B	2.870340	3.585848	3.531564	2.773883	2.299700																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 C	0.000000																																																																																																																																																
7 C	3.290009	0.000000																																																																																																																																															
8 B	1.708569	3.532888	0.000000																																																																																																																																														
9 B	3.494412	1.609999	2.921729	0.000000																																																																																																																																													
10 B	1.690108	2.876421	1.842829	2.911225	0.000000																																																																																																																																												
11 B	2.815063	2.763426	1.730431	1.773759	1.840249																																																																																																																																												
12 B	3.030849	1.659005	2.950061	1.817229	1.803721																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.794371	0.000000																																																																																																																																															

 <p>7. -578.48607003 +6.0</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>2.935936</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.765551</td><td>1.773110</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.738300</td><td>1.790588</td><td>1.760205</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>3.547347</td><td>1.604737</td><td>2.830415</td><td>2.770291</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.895711</td><td>1.920955</td><td>1.903137</td><td>2.875990</td><td>1.728472</td></tr> <tr><td>7 B</td><td>2.938416</td><td>1.840564</td><td>2.873746</td><td>1.795488</td><td>1.659466</td></tr> <tr><td>8 C</td><td>1.706912</td><td>2.950965</td><td>1.676512</td><td>2.784711</td><td>3.196668</td></tr> <tr><td>9 B</td><td>1.830648</td><td>2.918011</td><td>2.837864</td><td>1.846483</td><td>2.875771</td></tr> <tr><td>10 Re</td><td>3.395370</td><td>3.203366</td><td>3.590801</td><td>3.417789</td><td>2.019383</td></tr> <tr><td>11 B</td><td>2.938881</td><td>3.558024</td><td>3.005372</td><td>3.752442</td><td>2.981176</td></tr> <tr><td>12 B</td><td>1.782620</td><td>3.613311</td><td>2.867590</td><td>2.933740</td><td>3.401312</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.764539</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>1.839388</td><td>3.430698</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.108406</td><td>1.784749</td><td>2.748329</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>2.441657</td><td>2.325159</td><td>3.010767</td><td>2.301490</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.914761</td><td>3.593263</td><td>1.653388</td><td>3.043617</td><td>2.066201</td></tr> <tr><td>12 B</td><td>2.796584</td><td>3.117929</td><td>1.745911</td><td>1.761534</td><td>2.278379</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.777349</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.935936	0.000000				3 B	1.765551	1.773110	0.000000			4 B	1.738300	1.790588	1.760205	0.000000		5 C	3.547347	1.604737	2.830415	2.770291	0.000000	6 B	2.895711	1.920955	1.903137	2.875990	1.728472	7 B	2.938416	1.840564	2.873746	1.795488	1.659466	8 C	1.706912	2.950965	1.676512	2.784711	3.196668	9 B	1.830648	2.918011	2.837864	1.846483	2.875771	10 Re	3.395370	3.203366	3.590801	3.417789	2.019383	11 B	2.938881	3.558024	3.005372	3.752442	2.981176	12 B	1.782620	3.613311	2.867590	2.933740	3.401312		6	7	8	9	10	6 B	0.000000					7 B	2.764539	0.000000				8 C	1.839388	3.430698	0.000000			9 B	3.108406	1.784749	2.748329	0.000000		10 Re	2.441657	2.325159	3.010767	2.301490	0.000000	11 B	1.914761	3.593263	1.653388	3.043617	2.066201	12 B	2.796584	3.117929	1.745911	1.761534	2.278379		11	12				11 B	0.000000					12 B	1.777349	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	2.935936	0.000000																																																																																																																																															
3 B	1.765551	1.773110	0.000000																																																																																																																																														
4 B	1.738300	1.790588	1.760205	0.000000																																																																																																																																													
5 C	3.547347	1.604737	2.830415	2.770291	0.000000																																																																																																																																												
6 B	2.895711	1.920955	1.903137	2.875990	1.728472																																																																																																																																												
7 B	2.938416	1.840564	2.873746	1.795488	1.659466																																																																																																																																												
8 C	1.706912	2.950965	1.676512	2.784711	3.196668																																																																																																																																												
9 B	1.830648	2.918011	2.837864	1.846483	2.875771																																																																																																																																												
10 Re	3.395370	3.203366	3.590801	3.417789	2.019383																																																																																																																																												
11 B	2.938881	3.558024	3.005372	3.752442	2.981176																																																																																																																																												
12 B	1.782620	3.613311	2.867590	2.933740	3.401312																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	2.764539	0.000000																																																																																																																																															
8 C	1.839388	3.430698	0.000000																																																																																																																																														
9 B	3.108406	1.784749	2.748329	0.000000																																																																																																																																													
10 Re	2.441657	2.325159	3.010767	2.301490	0.000000																																																																																																																																												
11 B	1.914761	3.593263	1.653388	3.043617	2.066201																																																																																																																																												
12 B	2.796584	3.117929	1.745911	1.761534	2.278379																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.777349	0.000000																																																																																																																																															
 <p>8. -578.48309588 +7.9</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.676817</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.735980</td><td>1.774587</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.039670</td><td>2.781110</td><td>1.767958</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.781607</td><td>3.502505</td><td>3.012694</td><td>1.807397</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.750480</td><td>2.956533</td><td>3.436597</td><td>2.716428</td><td>1.770657</td></tr> <tr><td>7 B</td><td>1.727786</td><td>1.763483</td><td>1.763040</td><td>2.751610</td><td>2.914308</td></tr> <tr><td>8 B</td><td>1.711186</td><td>2.875914</td><td>2.901574</td><td>2.749802</td><td>1.754804</td></tr> <tr><td>9 B</td><td>1.733479</td><td>1.825350</td><td>2.882330</td><td>2.707898</td><td>3.001881</td></tr> <tr><td>10 B</td><td>2.762189</td><td>2.897222</td><td>1.812684</td><td>1.735855</td><td>1.821470</td></tr> <tr><td>11 Re</td><td>3.365108</td><td>3.513547</td><td>3.441851</td><td>2.044589</td><td>2.316196</td></tr> <tr><td>12 C</td><td>2.609561</td><td>1.668255</td><td>1.714828</td><td>1.757729</td><td>3.044923</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.927447</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.790609</td><td>1.781209</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.880170</td><td>2.927424</td><td>2.934191</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.902128</td><td>1.771232</td><td>1.799584</td><td>3.425581</td><td>0.000000</td></tr> <tr><td>11 Re</td><td>2.271516</td><td>4.052983</td><td>3.502941</td><td>2.231568</td><td>3.447618</td></tr> <tr><td>12 C</td><td>2.895489</td><td>2.762854</td><td>3.332073</td><td>1.679807</td><td>2.866488</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 C</td><td>2.272458</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.676817	0.000000				3 B	2.735980	1.774587	0.000000			4 B	3.039670	2.781110	1.767958	0.000000		5 B	2.781607	3.502505	3.012694	1.807397	0.000000	6 B	1.750480	2.956533	3.436597	2.716428	1.770657	7 B	1.727786	1.763483	1.763040	2.751610	2.914308	8 B	1.711186	2.875914	2.901574	2.749802	1.754804	9 B	1.733479	1.825350	2.882330	2.707898	3.001881	10 B	2.762189	2.897222	1.812684	1.735855	1.821470	11 Re	3.365108	3.513547	3.441851	2.044589	2.316196	12 C	2.609561	1.668255	1.714828	1.757729	3.044923		6	7	8	9	10	6 B	0.000000					7 B	2.927447	0.000000				8 B	1.790609	1.781209	0.000000			9 B	1.880170	2.927424	2.934191	0.000000		10 B	2.902128	1.771232	1.799584	3.425581	0.000000	11 Re	2.271516	4.052983	3.502941	2.231568	3.447618	12 C	2.895489	2.762854	3.332073	1.679807	2.866488		11	12				11 Re	0.000000					12 C	2.272458	0.000000			
	1	2	3	4	5																																																																																																																																												
1 C	0.000000																																																																																																																																																
2 B	1.676817	0.000000																																																																																																																																															
3 B	2.735980	1.774587	0.000000																																																																																																																																														
4 B	3.039670	2.781110	1.767958	0.000000																																																																																																																																													
5 B	2.781607	3.502505	3.012694	1.807397	0.000000																																																																																																																																												
6 B	1.750480	2.956533	3.436597	2.716428	1.770657																																																																																																																																												
7 B	1.727786	1.763483	1.763040	2.751610	2.914308																																																																																																																																												
8 B	1.711186	2.875914	2.901574	2.749802	1.754804																																																																																																																																												
9 B	1.733479	1.825350	2.882330	2.707898	3.001881																																																																																																																																												
10 B	2.762189	2.897222	1.812684	1.735855	1.821470																																																																																																																																												
11 Re	3.365108	3.513547	3.441851	2.044589	2.316196																																																																																																																																												
12 C	2.609561	1.668255	1.714828	1.757729	3.044923																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	2.927447	0.000000																																																																																																																																															
8 B	1.790609	1.781209	0.000000																																																																																																																																														
9 B	1.880170	2.927424	2.934191	0.000000																																																																																																																																													
10 B	2.902128	1.771232	1.799584	3.425581	0.000000																																																																																																																																												
11 Re	2.271516	4.052983	3.502941	2.231568	3.447618																																																																																																																																												
12 C	2.895489	2.762854	3.332073	1.679807	2.866488																																																																																																																																												
	11	12																																																																																																																																															
11 Re	0.000000																																																																																																																																																
12 C	2.272458	0.000000																																																																																																																																															

 <p>9. -578.48260346 +8.2</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 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.400523</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.277636</td><td>1.864384</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.252133</td><td>1.835161</td><td>1.796685</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.451126</td><td>1.790907</td><td>2.832479</td><td>2.791510</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.372794</td><td>1.723075</td><td>1.842283</td><td>2.937165</td><td>1.822144</td></tr> <tr><td>7 C</td><td>3.143095</td><td>1.624638</td><td>2.778997</td><td>1.681597</td><td>1.690251</td></tr> <tr><td>8 B</td><td>2.373611</td><td>2.966207</td><td>1.780557</td><td>3.172420</td><td>2.896178</td></tr> <tr><td>9 B</td><td>2.132264</td><td>2.840033</td><td>3.026513</td><td>1.792474</td><td>2.609159</td></tr> <tr><td>10 B</td><td>3.123749</td><td>2.971029</td><td>2.915670</td><td>3.607058</td><td>1.798989</td></tr> <tr><td>11 C</td><td>2.017403</td><td>3.691090</td><td>2.881177</td><td>3.510520</td><td>2.936533</td></tr> <tr><td>12 B</td><td>2.296269</td><td>3.134401</td><td>3.144235</td><td>2.955029</td><td>1.987010</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 C</td><td>2.824229</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.772818</td><td>3.622885</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.570502</td><td>1.609016</td><td>3.577437</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.820639</td><td>3.154211</td><td>1.852054</td><td>3.320100</td><td>0.000000</td></tr> <tr><td>11 C</td><td>2.807834</td><td>3.628671</td><td>1.636590</td><td>3.053551</td><td>1.640576</td></tr> <tr><td>12 B</td><td>2.908630</td><td>2.432974</td><td>2.690693</td><td>1.879860</td><td>1.775706</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.666932</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 Re	0.000000					2 B	3.400523	0.000000				3 B	2.277636	1.864384	0.000000			4 B	2.252133	1.835161	1.796685	0.000000		5 B	3.451126	1.790907	2.832479	2.791510	0.000000	6 B	3.372794	1.723075	1.842283	2.937165	1.822144	7 C	3.143095	1.624638	2.778997	1.681597	1.690251	8 B	2.373611	2.966207	1.780557	3.172420	2.896178	9 B	2.132264	2.840033	3.026513	1.792474	2.609159	10 B	3.123749	2.971029	2.915670	3.607058	1.798989	11 C	2.017403	3.691090	2.881177	3.510520	2.936533	12 B	2.296269	3.134401	3.144235	2.955029	1.987010		6	7	8	9	10	6 B	0.000000					7 C	2.824229	0.000000				8 B	1.772818	3.622885	0.000000			9 B	3.570502	1.609016	3.577437	0.000000		10 B	1.820639	3.154211	1.852054	3.320100	0.000000	11 C	2.807834	3.628671	1.636590	3.053551	1.640576	12 B	2.908630	2.432974	2.690693	1.879860	1.775706		11	12				11 C	0.000000					12 B	1.666932	0.000000			
	1	2	3	4	5																																																																																																																																												
1 Re	0.000000																																																																																																																																																
2 B	3.400523	0.000000																																																																																																																																															
3 B	2.277636	1.864384	0.000000																																																																																																																																														
4 B	2.252133	1.835161	1.796685	0.000000																																																																																																																																													
5 B	3.451126	1.790907	2.832479	2.791510	0.000000																																																																																																																																												
6 B	3.372794	1.723075	1.842283	2.937165	1.822144																																																																																																																																												
7 C	3.143095	1.624638	2.778997	1.681597	1.690251																																																																																																																																												
8 B	2.373611	2.966207	1.780557	3.172420	2.896178																																																																																																																																												
9 B	2.132264	2.840033	3.026513	1.792474	2.609159																																																																																																																																												
10 B	3.123749	2.971029	2.915670	3.607058	1.798989																																																																																																																																												
11 C	2.017403	3.691090	2.881177	3.510520	2.936533																																																																																																																																												
12 B	2.296269	3.134401	3.144235	2.955029	1.987010																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 C	2.824229	0.000000																																																																																																																																															
8 B	1.772818	3.622885	0.000000																																																																																																																																														
9 B	3.570502	1.609016	3.577437	0.000000																																																																																																																																													
10 B	1.820639	3.154211	1.852054	3.320100	0.000000																																																																																																																																												
11 C	2.807834	3.628671	1.636590	3.053551	1.640576																																																																																																																																												
12 B	2.908630	2.432974	2.690693	1.879860	1.775706																																																																																																																																												
	11	12																																																																																																																																															
11 C	0.000000																																																																																																																																																
12 B	1.666932	0.000000																																																																																																																																															
 <p>10. -578.48148763 +8.9</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 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.764495</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.643244</td><td>1.758180</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.696728</td><td>1.732109</td><td>1.762204</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.573269</td><td>1.746274</td><td>2.925327</td><td>3.005250</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.688135</td><td>1.714844</td><td>1.692756</td><td>2.732306</td><td>1.697137</td></tr> <tr><td>7 B</td><td>2.750344</td><td>1.897986</td><td>2.861592</td><td>1.870043</td><td>1.892279</td></tr> <tr><td>8 B</td><td>1.792837</td><td>2.871447</td><td>1.866146</td><td>2.868975</td><td>2.955927</td></tr> <tr><td>9 B</td><td>1.693946</td><td>3.057958</td><td>2.887284</td><td>1.759311</td><td>3.535519</td></tr> <tr><td>10 Re</td><td>3.259640</td><td>3.179792</td><td>3.395223</td><td>3.597982</td><td>2.054444</td></tr> <tr><td>11 B</td><td>1.716021</td><td>3.571750</td><td>2.923846</td><td>2.861075</td><td>3.548607</td></tr> <tr><td>12 B</td><td>2.831799</td><td>3.507305</td><td>3.722431</td><td>2.995209</td><td>3.066259</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.653145</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.698100</td><td>3.096672</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.457092</td><td>1.963809</td><td>2.888378</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>2.272329</td><td>2.491598</td><td>2.216810</td><td>3.178411</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.040341</td><td>2.789098</td><td>1.791009</td><td>1.783015</td><td>2.298215</td></tr> <tr><td>12 B</td><td>3.463935</td><td>1.908660</td><td>3.003876</td><td>1.732829</td><td>2.072901</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.755840</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	2.764495	0.000000				3 B	1.643244	1.758180	0.000000			4 B	1.696728	1.732109	1.762204	0.000000		5 B	3.573269	1.746274	2.925327	3.005250	0.000000	6 C	2.688135	1.714844	1.692756	2.732306	1.697137	7 B	2.750344	1.897986	2.861592	1.870043	1.892279	8 B	1.792837	2.871447	1.866146	2.868975	2.955927	9 B	1.693946	3.057958	2.887284	1.759311	3.535519	10 Re	3.259640	3.179792	3.395223	3.597982	2.054444	11 B	1.716021	3.571750	2.923846	2.861075	3.548607	12 B	2.831799	3.507305	3.722431	2.995209	3.066259		6	7	8	9	10	6 C	0.000000					7 B	2.653145	0.000000				8 B	1.698100	3.096672	0.000000			9 B	3.457092	1.963809	2.888378	0.000000		10 Re	2.272329	2.491598	2.216810	3.178411	0.000000	11 B	3.040341	2.789098	1.791009	1.783015	2.298215	12 B	3.463935	1.908660	3.003876	1.732829	2.072901		11	12				11 B	0.000000					12 B	1.755840	0.000000			
	1	2	3	4	5																																																																																																																																												
1 C	0.000000																																																																																																																																																
2 B	2.764495	0.000000																																																																																																																																															
3 B	1.643244	1.758180	0.000000																																																																																																																																														
4 B	1.696728	1.732109	1.762204	0.000000																																																																																																																																													
5 B	3.573269	1.746274	2.925327	3.005250	0.000000																																																																																																																																												
6 C	2.688135	1.714844	1.692756	2.732306	1.697137																																																																																																																																												
7 B	2.750344	1.897986	2.861592	1.870043	1.892279																																																																																																																																												
8 B	1.792837	2.871447	1.866146	2.868975	2.955927																																																																																																																																												
9 B	1.693946	3.057958	2.887284	1.759311	3.535519																																																																																																																																												
10 Re	3.259640	3.179792	3.395223	3.597982	2.054444																																																																																																																																												
11 B	1.716021	3.571750	2.923846	2.861075	3.548607																																																																																																																																												
12 B	2.831799	3.507305	3.722431	2.995209	3.066259																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 C	0.000000																																																																																																																																																
7 B	2.653145	0.000000																																																																																																																																															
8 B	1.698100	3.096672	0.000000																																																																																																																																														
9 B	3.457092	1.963809	2.888378	0.000000																																																																																																																																													
10 Re	2.272329	2.491598	2.216810	3.178411	0.000000																																																																																																																																												
11 B	3.040341	2.789098	1.791009	1.783015	2.298215																																																																																																																																												
12 B	3.463935	1.908660	3.003876	1.732829	2.072901																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.755840	0.000000																																																																																																																																															

 <p>11. -578.48052841 +9.5</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>3.105613</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.906125</td><td>2.978568</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.846766</td><td>2.869167</td><td>1.748324</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.871695</td><td>1.858910</td><td>2.945381</td><td>1.775739</td><td>0.000000</td></tr> <tr><td>6 C</td><td>2.624463</td><td>1.695608</td><td>1.682798</td><td>1.720595</td><td>1.699449</td></tr> <tr><td>7 B</td><td>1.855438</td><td>3.029100</td><td>3.083498</td><td>3.422424</td><td>3.697630</td></tr> <tr><td>8 B</td><td>2.804737</td><td>1.780931</td><td>3.561743</td><td>3.549133</td><td>2.932099</td></tr> <tr><td>9 C</td><td>1.945169</td><td>2.759095</td><td>3.481315</td><td>2.939557</td><td>2.779909</td></tr> <tr><td>10 B</td><td>2.932147</td><td>1.842656</td><td>3.762594</td><td>2.903811</td><td>1.728380</td></tr> <tr><td>11 B</td><td>1.904016</td><td>2.846964</td><td>3.060667</td><td>1.746006</td><td>1.762145</td></tr> <tr><td>12 Re</td><td>2.440590</td><td>2.275230</td><td>2.052190</td><td>3.152007</td><td>3.419865</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.437054</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.010961</td><td>1.780233</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.317740</td><td>1.649610</td><td>1.716910</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.806009</td><td>2.920539</td><td>1.781984</td><td>1.687300</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.733371</td><td>2.916287</td><td>2.847416</td><td>1.673976</td><td>1.782857</td></tr> <tr><td>12 Re</td><td>2.281954</td><td>2.073562</td><td>2.276205</td><td>3.058709</td><td>3.396650</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Re</td><td>3.583753</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	3.105613	0.000000				3 B	1.906125	2.978568	0.000000			4 B	1.846766	2.869167	1.748324	0.000000		5 B	2.871695	1.858910	2.945381	1.775739	0.000000	6 C	2.624463	1.695608	1.682798	1.720595	1.699449	7 B	1.855438	3.029100	3.083498	3.422424	3.697630	8 B	2.804737	1.780931	3.561743	3.549133	2.932099	9 C	1.945169	2.759095	3.481315	2.939557	2.779909	10 B	2.932147	1.842656	3.762594	2.903811	1.728380	11 B	1.904016	2.846964	3.060667	1.746006	1.762145	12 Re	2.440590	2.275230	2.052190	3.152007	3.419865		6	7	8	9	10	6 C	0.000000					7 B	3.437054	0.000000				8 B	3.010961	1.780233	0.000000			9 C	3.317740	1.649610	1.716910	0.000000		10 B	2.806009	2.920539	1.781984	1.687300	0.000000	11 B	2.733371	2.916287	2.847416	1.673976	1.782857	12 Re	2.281954	2.073562	2.276205	3.058709	3.396650		11	12				11 B	0.000000					12 Re	3.583753	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	3.105613	0.000000																																																																																																																																															
3 B	1.906125	2.978568	0.000000																																																																																																																																														
4 B	1.846766	2.869167	1.748324	0.000000																																																																																																																																													
5 B	2.871695	1.858910	2.945381	1.775739	0.000000																																																																																																																																												
6 C	2.624463	1.695608	1.682798	1.720595	1.699449																																																																																																																																												
7 B	1.855438	3.029100	3.083498	3.422424	3.697630																																																																																																																																												
8 B	2.804737	1.780931	3.561743	3.549133	2.932099																																																																																																																																												
9 C	1.945169	2.759095	3.481315	2.939557	2.779909																																																																																																																																												
10 B	2.932147	1.842656	3.762594	2.903811	1.728380																																																																																																																																												
11 B	1.904016	2.846964	3.060667	1.746006	1.762145																																																																																																																																												
12 Re	2.440590	2.275230	2.052190	3.152007	3.419865																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 C	0.000000																																																																																																																																																
7 B	3.437054	0.000000																																																																																																																																															
8 B	3.010961	1.780233	0.000000																																																																																																																																														
9 C	3.317740	1.649610	1.716910	0.000000																																																																																																																																													
10 B	2.806009	2.920539	1.781984	1.687300	0.000000																																																																																																																																												
11 B	2.733371	2.916287	2.847416	1.673976	1.782857																																																																																																																																												
12 Re	2.281954	2.073562	2.276205	3.058709	3.396650																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 Re	3.583753	0.000000																																																																																																																																															
 <p>12. -578.48001896 +9.8</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>3.016263</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.753482</td><td>1.735337</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.853274</td><td>1.915923</td><td>1.902382</td><td>0.000000</td><td></td></tr> <tr><td>5 Re</td><td>3.568300</td><td>2.072290</td><td>3.165391</td><td>2.463741</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.850712</td><td>1.753200</td><td>1.803181</td><td>2.765157</td><td>2.314384</td></tr> <tr><td>7 B</td><td>2.944078</td><td>3.087798</td><td>3.488735</td><td>1.867318</td><td>2.074933</td></tr> <tr><td>8 C</td><td>1.676195</td><td>2.834240</td><td>1.700529</td><td>2.718404</td><td>3.262392</td></tr> <tr><td>9 C</td><td>1.663328</td><td>3.431107</td><td>2.948677</td><td>1.853262</td><td>3.045430</td></tr> <tr><td>10 B</td><td>2.864724</td><td>3.023635</td><td>2.908617</td><td>3.110200</td><td>2.252122</td></tr> <tr><td>11 B</td><td>1.789963</td><td>3.740807</td><td>2.911334</td><td>2.877238</td><td>3.363138</td></tr> <tr><td>12 B</td><td>2.864202</td><td>3.588133</td><td>3.595387</td><td>2.794677</td><td>2.288772</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>3.562732</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 C</td><td>1.712160</td><td>3.561039</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.439705</td><td>1.657480</td><td>2.649079</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.785520</td><td>3.017806</td><td>1.801001</td><td>2.765727</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.903690</td><td>2.911041</td><td>1.652825</td><td>1.696733</td><td>1.829461</td></tr> <tr><td>12 B</td><td>3.131374</td><td>1.779153</td><td>2.817050</td><td>1.745045</td><td>1.768274</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.766205</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	3.016263	0.000000				3 B	1.753482	1.735337	0.000000			4 B	1.853274	1.915923	1.902382	0.000000		5 Re	3.568300	2.072290	3.165391	2.463741	0.000000	6 B	2.850712	1.753200	1.803181	2.765157	2.314384	7 B	2.944078	3.087798	3.488735	1.867318	2.074933	8 C	1.676195	2.834240	1.700529	2.718404	3.262392	9 C	1.663328	3.431107	2.948677	1.853262	3.045430	10 B	2.864724	3.023635	2.908617	3.110200	2.252122	11 B	1.789963	3.740807	2.911334	2.877238	3.363138	12 B	2.864202	3.588133	3.595387	2.794677	2.288772		6	7	8	9	10	6 B	0.000000					7 B	3.562732	0.000000				8 C	1.712160	3.561039	0.000000			9 C	3.439705	1.657480	2.649079	0.000000		10 B	1.785520	3.017806	1.801001	2.765727	0.000000	11 B	2.903690	2.911041	1.652825	1.696733	1.829461	12 B	3.131374	1.779153	2.817050	1.745045	1.768274		11	12				11 B	0.000000					12 B	1.766205	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 B	3.016263	0.000000																																																																																																																																															
3 B	1.753482	1.735337	0.000000																																																																																																																																														
4 B	1.853274	1.915923	1.902382	0.000000																																																																																																																																													
5 Re	3.568300	2.072290	3.165391	2.463741	0.000000																																																																																																																																												
6 B	2.850712	1.753200	1.803181	2.765157	2.314384																																																																																																																																												
7 B	2.944078	3.087798	3.488735	1.867318	2.074933																																																																																																																																												
8 C	1.676195	2.834240	1.700529	2.718404	3.262392																																																																																																																																												
9 C	1.663328	3.431107	2.948677	1.853262	3.045430																																																																																																																																												
10 B	2.864724	3.023635	2.908617	3.110200	2.252122																																																																																																																																												
11 B	1.789963	3.740807	2.911334	2.877238	3.363138																																																																																																																																												
12 B	2.864202	3.588133	3.595387	2.794677	2.288772																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	3.562732	0.000000																																																																																																																																															
8 C	1.712160	3.561039	0.000000																																																																																																																																														
9 C	3.439705	1.657480	2.649079	0.000000																																																																																																																																													
10 B	1.785520	3.017806	1.801001	2.765727	0.000000																																																																																																																																												
11 B	2.903690	2.911041	1.652825	1.696733	1.829461																																																																																																																																												
12 B	3.131374	1.779153	2.817050	1.745045	1.768274																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 B	1.766205	0.000000																																																																																																																																															

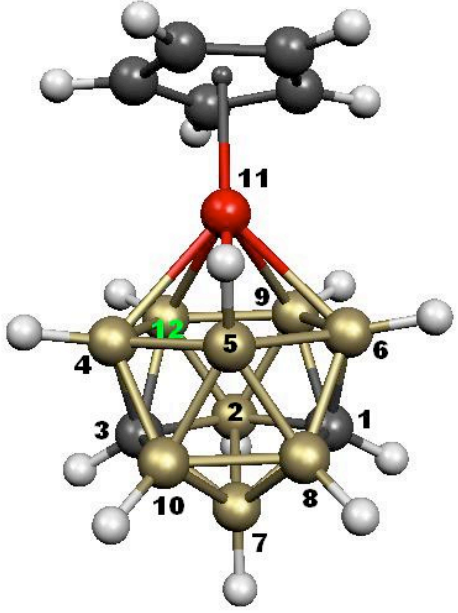
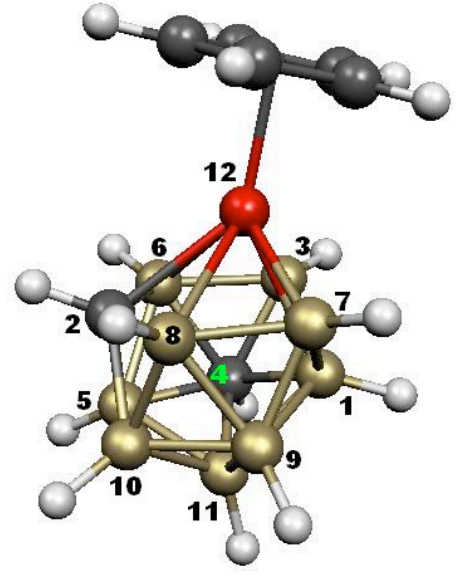
 <p>13. -578.47786391 +11.1 Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.693238</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>2.634084</td><td>1.691641</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.338879</td><td>2.884505</td><td>1.708677</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.655956</td><td>3.205344</td><td>2.655758</td><td>1.806685</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.710072</td><td>2.888290</td><td>3.340236</td><td>3.124688</td><td>1.805727</td></tr> <tr><td>7 B</td><td>1.694094</td><td>1.797982</td><td>1.693646</td><td>2.896274</td><td>2.755296</td></tr> <tr><td>8 B</td><td>1.709587</td><td>2.869765</td><td>2.775279</td><td>2.986961</td><td>1.759320</td></tr> <tr><td>9 B</td><td>1.743851</td><td>1.778282</td><td>2.812829</td><td>3.010585</td><td>2.764408</td></tr> <tr><td>10 B</td><td>2.774962</td><td>2.868179</td><td>1.708354</td><td>1.802383</td><td>1.758639</td></tr> <tr><td>11 Re</td><td>3.364302</td><td>3.446773</td><td>3.369022</td><td>2.276982</td><td>2.042037</td></tr> <tr><td>12 B</td><td>2.812056</td><td>1.778462</td><td>1.748284</td><td>1.814942</td><td>2.763601</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.896825</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.801599</td><td>1.757719</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.817053</td><td>2.914092</td><td>2.913226</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.985746</td><td>1.757380</td><td>1.814944</td><td>3.440275</td><td>0.000000</td></tr> <tr><td>11 Re</td><td>2.270562</td><td>4.014473</td><td>3.424371</td><td>2.252194</td><td>3.426469</td></tr> <tr><td>12 B</td><td>3.010814</td><td>2.916232</td><td>3.441397</td><td>1.845456</td><td>2.914280</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>2.253236</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 C	0.000000					2 B	1.693238	0.000000				3 C	2.634084	1.691641	0.000000			4 B	3.338879	2.884505	1.708677	0.000000		5 B	2.655956	3.205344	2.655758	1.806685	0.000000	6 B	1.710072	2.888290	3.340236	3.124688	1.805727	7 B	1.694094	1.797982	1.693646	2.896274	2.755296	8 B	1.709587	2.869765	2.775279	2.986961	1.759320	9 B	1.743851	1.778282	2.812829	3.010585	2.764408	10 B	2.774962	2.868179	1.708354	1.802383	1.758639	11 Re	3.364302	3.446773	3.369022	2.276982	2.042037	12 B	2.812056	1.778462	1.748284	1.814942	2.763601		6	7	8	9	10	6 B	0.000000					7 B	2.896825	0.000000				8 B	1.801599	1.757719	0.000000			9 B	1.817053	2.914092	2.913226	0.000000		10 B	2.985746	1.757380	1.814944	3.440275	0.000000	11 Re	2.270562	4.014473	3.424371	2.252194	3.426469	12 B	3.010814	2.916232	3.441397	1.845456	2.914280		11	12				11 Re	0.000000					12 B	2.253236	0.000000			
	1	2	3	4	5																																																																																																																																												
1 C	0.000000																																																																																																																																																
2 B	1.693238	0.000000																																																																																																																																															
3 C	2.634084	1.691641	0.000000																																																																																																																																														
4 B	3.338879	2.884505	1.708677	0.000000																																																																																																																																													
5 B	2.655956	3.205344	2.655758	1.806685	0.000000																																																																																																																																												
6 B	1.710072	2.888290	3.340236	3.124688	1.805727																																																																																																																																												
7 B	1.694094	1.797982	1.693646	2.896274	2.755296																																																																																																																																												
8 B	1.709587	2.869765	2.775279	2.986961	1.759320																																																																																																																																												
9 B	1.743851	1.778282	2.812829	3.010585	2.764408																																																																																																																																												
10 B	2.774962	2.868179	1.708354	1.802383	1.758639																																																																																																																																												
11 Re	3.364302	3.446773	3.369022	2.276982	2.042037																																																																																																																																												
12 B	2.812056	1.778462	1.748284	1.814942	2.763601																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	2.896825	0.000000																																																																																																																																															
8 B	1.801599	1.757719	0.000000																																																																																																																																														
9 B	1.817053	2.914092	2.913226	0.000000																																																																																																																																													
10 B	2.985746	1.757380	1.814944	3.440275	0.000000																																																																																																																																												
11 Re	2.270562	4.014473	3.424371	2.252194	3.426469																																																																																																																																												
12 B	3.010814	2.916232	3.441397	1.845456	2.914280																																																																																																																																												
	11	12																																																																																																																																															
11 Re	0.000000																																																																																																																																																
12 B	2.253236	0.000000																																																																																																																																															
 <p>14. -578.47780020 +11.2</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 C</td><td>2.953883</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.852814</td><td>2.925622</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.878999</td><td>2.612569</td><td>1.646553</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.869178</td><td>1.741382</td><td>2.917617</td><td>1.673245</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.775039</td><td>1.682284</td><td>1.783427</td><td>1.738623</td><td>1.802308</td></tr> <tr><td>7 B</td><td>1.916378</td><td>2.929414</td><td>3.075558</td><td>3.452437</td><td>3.757403</td></tr> <tr><td>8 B</td><td>2.761194</td><td>1.691360</td><td>3.538580</td><td>3.433559</td><td>2.907461</td></tr> <tr><td>9 B</td><td>1.886316</td><td>2.752764</td><td>3.464535</td><td>2.964263</td><td>2.903635</td></tr> <tr><td>10 B</td><td>2.849676</td><td>1.765303</td><td>3.707556</td><td>2.778591</td><td>1.724862</td></tr> <tr><td>11 B</td><td>1.874089</td><td>2.699354</td><td>2.952555</td><td>1.698302</td><td>1.762026</td></tr> <tr><td>12 Re</td><td>2.466432</td><td>2.253066</td><td>2.076328</td><td>3.052919</td><td>3.406644</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>3.545825</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.055258</td><td>1.770880</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.558012</td><td>1.736837</td><td>1.823235</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.924822</td><td>2.958728</td><td>1.794638</td><td>1.768772</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.874328</td><td>3.046829</td><td>2.868482</td><td>1.765167</td><td>1.747313</td></tr> <tr><td>12 Re</td><td>2.251853</td><td>2.069802</td><td>2.305979</td><td>3.165846</td><td>3.428463</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Re</td><td>3.603637</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 C	2.953883	0.000000				3 B	1.852814	2.925622	0.000000			4 C	1.878999	2.612569	1.646553	0.000000		5 B	2.869178	1.741382	2.917617	1.673245	0.000000	6 B	2.775039	1.682284	1.783427	1.738623	1.802308	7 B	1.916378	2.929414	3.075558	3.452437	3.757403	8 B	2.761194	1.691360	3.538580	3.433559	2.907461	9 B	1.886316	2.752764	3.464535	2.964263	2.903635	10 B	2.849676	1.765303	3.707556	2.778591	1.724862	11 B	1.874089	2.699354	2.952555	1.698302	1.762026	12 Re	2.466432	2.253066	2.076328	3.052919	3.406644		6	7	8	9	10	6 B	0.000000					7 B	3.545825	0.000000				8 B	3.055258	1.770880	0.000000			9 B	3.558012	1.736837	1.823235	0.000000		10 B	2.924822	2.958728	1.794638	1.768772	0.000000	11 B	2.874328	3.046829	2.868482	1.765167	1.747313	12 Re	2.251853	2.069802	2.305979	3.165846	3.428463		11	12				11 B	0.000000					12 Re	3.603637	0.000000			
	1	2	3	4	5																																																																																																																																												
1 B	0.000000																																																																																																																																																
2 C	2.953883	0.000000																																																																																																																																															
3 B	1.852814	2.925622	0.000000																																																																																																																																														
4 C	1.878999	2.612569	1.646553	0.000000																																																																																																																																													
5 B	2.869178	1.741382	2.917617	1.673245	0.000000																																																																																																																																												
6 B	2.775039	1.682284	1.783427	1.738623	1.802308																																																																																																																																												
7 B	1.916378	2.929414	3.075558	3.452437	3.757403																																																																																																																																												
8 B	2.761194	1.691360	3.538580	3.433559	2.907461																																																																																																																																												
9 B	1.886316	2.752764	3.464535	2.964263	2.903635																																																																																																																																												
10 B	2.849676	1.765303	3.707556	2.778591	1.724862																																																																																																																																												
11 B	1.874089	2.699354	2.952555	1.698302	1.762026																																																																																																																																												
12 Re	2.466432	2.253066	2.076328	3.052919	3.406644																																																																																																																																												
	6	7	8	9	10																																																																																																																																												
6 B	0.000000																																																																																																																																																
7 B	3.545825	0.000000																																																																																																																																															
8 B	3.055258	1.770880	0.000000																																																																																																																																														
9 B	3.558012	1.736837	1.823235	0.000000																																																																																																																																													
10 B	2.924822	2.958728	1.794638	1.768772	0.000000																																																																																																																																												
11 B	2.874328	3.046829	2.868482	1.765167	1.747313																																																																																																																																												
12 Re	2.251853	2.069802	2.305979	3.165846	3.428463																																																																																																																																												
	11	12																																																																																																																																															
11 B	0.000000																																																																																																																																																
12 Re	3.603637	0.000000																																																																																																																																															

Table 4. Energy ranking

No	Initial structure	Final energy (a.u.)	D kcal/mole	Remarks
1	2-Cuboctaedru_Re_v4_C2_x	-578.49560700	0.00	
2	3-Anticuboh_Re_v6_C2_q	-578.49560700	0.00	
3	2-Cuboctaedru_Re_v6_C2_n	-578.49560699	0.00	
4	3-Anticuboh_Re_v4_C2_j	-578.49560699	0.00	
5	3-Anticuboh_Re_v5_C2_y	-578.49560699	0.00	
6	3-Anticuboh_Re_v6_C2_f	-578.49560699	0.00	
7	3-Anticuboh_Re_v5_C2_f	-578.49406073	0.97	
8	2-Cuboctaedru_Re_v4_C2_za	-578.49406072	0.97	
9	2-Cuboctaedru_Re_v6_C2_m	-578.49406071	0.97	
10	3-Anticuboh_Re_v5_C2_n	-578.49406071	0.97	
11	3-Anticuboh_Re_v5_C2_s	-578.49406071	0.97	
12	3-Anticuboh_Re_v6_C2_h	-578.49406071	0.97	
13	3-Anticuboh_Re_v4_C2_l	-578.49406070	0.97	
14	3-Anticuboh_Re_v6_C2_n	-578.49027655	3.34	
15	2-Cuboctaedru_Re_v4_C2_n	-578.49027654	3.34	C-C
16	2-Cuboctaedru_Re_v4_C2_w	-578.48957885	3.78	
17	3-Anticuboh_Re_v5_C2_c_r-33	-578.48957885	3.78	
18	3-Anticuboh_Re_v6_C2_b	-578.48957885	3.78	
19	2-Cuboctaedru_Re_v4_C2_d	-578.48906733	4.10	C-C
20	2-Cuboctaedru_Re_v6_C2_g	-578.48906733	4.10	
21	3-Anticuboh_Re_v4_C2_m	-578.48906733	4.10	
22	3-Anticuboh_Re_v4_C2_q	-578.48906733	4.10	
23	3-Anticuboh_Re_v6_C2_r	-578.48906732	4.10	
24	3-Anticuboh_Re_v5_C2_c_i-33	-578.48869334	4.34	
25	3-Anticuboh_Re_v4_C2_n	-578.48854849	4.43	
26	2-Cuboctaedru_Re_v4_C2_q	-578.48854848	4.43	
27	2-Cuboctaedru_Re_v6_C2_q	-578.48854848	4.43	
28	3-Anticuboh_Re_v5_C2_u	-578.48854848	4.43	
29	3-Anticuboh_Re_v6_C2_s	-578.48854848	4.43	
30	3-Anticuboh_Re_v5_C2_e	-578.48607003	5.98	
31	3-Anticuboh_Re_v5_C2_j	-578.48607001	5.98	
32	3-Anticuboh_Re_v6_C2_e	-578.48607001	5.98	
33	2-Cuboctaedru_Re_v4_C2_y	-578.48607000	5.98	
34	2-Cuboctaedru_Re_v6_C2_o	-578.48607000	5.98	
35	3-Anticuboh_Re_v4_C2_k	-578.48607000	5.98	
36	1-Icos_Re_C2_f	-578.48309588	7.85	
37	3-Anticuboh_Re_v6_C2_i	-578.48260346	8.16	
38	3-Anticuboh_Re_v5_C2_o	-578.48148763	8.86	

39	3-Anticuboh_Re_v5_C2_x	-578.48148762	8.86	
40	2-Cuboctaedru_Re_v4_C2_r	-578.48134611	8.95	
41	2-Cuboctaedru_Re_v4_C2_s	-578.48052841	9.46	
42	3-Anticuboh_Re_v5_C2_t	-578.48052841	9.46	
43	3-Anticuboh_Re_v4_C2_g_r-188	-578.48001896	9.78	
44	3-Anticuboh_Re_v6_C2_k_r-188	-578.48001896	9.78	
45	3-Anticuboh_Re_v4_C2_t	-578.47994967	9.82	
46	2-Cuboctaedru_Re_v4_C2_zc	-578.47994966	9.82	
47	2-Cuboctaedru_Re_v6_C2_j	-578.47994966	9.82	
48	1-Icos_Re_C2_d_r-23	-578.47786391	11.13	
49	1-Icos_Re_C2_d_i-23	-578.47781308	11.17	
50	2-Cuboctaedru_Re_v4_C2_f	-578.47780020	11.17	
51	3-Anticuboh_Re_v5_C2_k	-578.47780020	11.17	
52	2-Cuboctaedru_Re_v6_C2_e	-578.47780019	11.17	
53	3-Anticuboh_Re_v5_C2_l	-578.47773119	11.22	
54	3-Anticuboh_Re_v6_C2_j	-578.47773119	11.22	
55	2-Cuboctaedru_Re_v4_C2_ze	-578.47770341	11.23	
56	2-Cuboctaedru_Re_v4_C2_zb	-578.47766191	11.26	
57	3-Anticuboh_Re_v4_C2_s_calcfc	-578.47740634	11.42	
58	1-Icos_Re_C2_i	-578.47736427	11.45	
59	2-Cuboctaedru_Re_v4_C2_p	-578.47669291	11.87	
60	2-Cuboctaedru_Re_v6_C2_p	-578.47669291	11.87	
61	3-Anticuboh_Re_v5_C2_p	-578.47669291	11.87	
62	2-Cuboctaedru_Re_v4_C2_b	-578.47613167	12.22	
63	2-Cuboctaedru_Re_v6_C2_c	-578.47613167	12.22	
64	3-Anticuboh_Re_v4_C2_b	-578.47604666	12.27	
65	2-Cuboctaedru_Re_v4_C2_o	-578.47585941	12.39	
66	3-Anticuboh_Re_v5_C2_zc	-578.47532446	12.73	
67	1-Icos_Re_C2_b	-578.47232669	14.61	
68	3-Anticuboh_Re_v4_C2_p	-578.46815449	17.23	
69	2-Cuboctaedru_Re_v6_C2_b	-578.46795582	17.35	
70	3-Anticuboh_Re_v4_C2_c	-578.46795582	17.35	
71	3-Anticuboh_Re_v6_C2_g	-578.46795582	17.35	
72	3-Anticuboh_Re_v5_C2_i	-578.46662806	18.18	
73	2-Cuboctaedru_Re_v4_C2_k	-578.46466348	19.42	
74	3-Anticuboh_Re_v4_C2_i	-578.46425564	19.67	
75	2-Cuboctaedru_Re_v4_C2_z	-578.46422084	19.69	
76	3-Anticuboh_Re_v4_C2_h	-578.46422084	19.69	
77	3-Anticuboh_Re_v5_C2_a	-578.46422084	19.69	C-C
78	2-Cuboctaedru_Re_v4_C2_v	-578.46343686	20.19	C-C
79	2-Cuboctaedru_Re_v6_C2_r	-578.46343686	20.19	C-C

80	3-Anticuboh_Re_v5_C2_d	-578.46343686	20.19	
81	3-Anticuboh_Re_v6_C2_a	-578.46343686	20.19	
82	1-Icos_Re_C2_g	-578.46172243	21.26	
83	2-Cuboctaedru_Re_v4_C2_j	-578.46126509	21.55	
84	2-Cuboctaedru_Re_v4_C2_i	-578.46064667	21.94	C-C
85	3-Anticuboh_Re_v6_C2_t	-578.46064667	21.94	C-C
86	3-Anticuboh_Re_v4_C2_e	-578.45997705	22.36	C-C
87	1-Icos_Re_C2_c_r-214	-578.45996797	22.36	C-C
88	3-Anticuboh_Re_v5_C2_l	-578.45991098	22.40	
89	3-Anticuboh_Re_v4_C2_s_calcall	-578.45974128	22.51	
90	2-Cuboctaedru_Re_v6_C2_k	-578.45942579	22.70	C-C
91	2-Cuboctaedru_Re_v4_C2_e	-578.45923006	22.83	C-C
92	2-Cuboctaedru_Re_v6_C2_d	-578.45923006	22.83	C-C
93	3-Anticuboh_Re_v5_C2_v	-578.45759525	23.85	
94	2-Cuboctaedru_Re_v4_C2_m	-578.45694321	24.26	C-C
95	2-Cuboctaedru_Re_v6_C2_a	-578.45694321	24.26	C-C
96	3-Anticuboh_Re_v4_C2_a_r-90	-578.45694321	24.26	C-C
97	1-Icos_Re_C2_a_i-12	-578.45692460	24.27	C-C
98	1-Icos_Re_C2_a_r-12	-578.45692460	24.27	C-C
99	2-Cuboctaedru_Re_v4_C2_u	-578.45654750	24.51	C-C
100	2-Cuboctaedru_Re_v6_C2_l	-578.45654750	24.51	C-C
101	3-Anticuboh_Re_v5_C2_r	-578.45654750	24.51	C-C
102	2-Cuboctaedru_Re_v4_C2_zd	-578.45639017	24.61	C-C
103	2-Cuboctaedru_Re_v6_C2_i	-578.45639015	24.61	C-C
104	1-Icos_Re_C2_h_r-52	-578.45481040	25.60	C-C
105	1-Icos_Re_C2_e	-578.45408253	26.06	C-C
106	2-Cuboctaedru_Re_v4_C2_l	-578.45326512	26.57	C-C
107	3-Anticuboh_Re_v5_C2_za	-578.45326512	26.57	C-C
108	3-Anticuboh_Re_v6_C2_m	-578.45326512	26.57	C-C
109	1-Icos_Re_C2_h_i-52	-578.45241683	27.10	C-C
110	3-Anticuboh_Re_v5_C2_w	-578.45068042	28.19	
111	2-Cuboctaedru_Re_v6_C2_f	-578.45068041	28.19	C-C
112	3-Anticuboh_Re_v5_C2_q	-578.45068041	28.19	C-C
113	2-Cuboctaedru_Re_v4_C2_c	-578.45068040	28.19	C-C
114	2-Cuboctaedru_Re_v4_C2_a	-578.44991498	28.67	
115	2-Cuboctaedru_Re_v6_C2_h	-578.44991498	28.67	
116	3-Anticuboh_Re_v5_C2_zb	-578.44922322	29.11	
117	2-Cuboctaedru_Re_v4_C2_g	-578.44879562	29.37	
118	2-Cuboctaedru_Re_v4_C2_h	-578.44661239	30.74	
119	3-Anticuboh_Re_v6_C2_c	-578.44482595	31.87	
120	1-Icos_Re_C2_c_i-214	-578.44481798	31.87	C-C

121	3-Anticuboh_Re_v4_C2_o	-578.44380041	32.51	C-C
122	3-Anticuboh_Re_v4_C2_d_r-34	-578.44265988	33.22	
123	3-Anticuboh_Re_v4_C2_d_r-81	-578.44265986	33.22	
124	3-Anticuboh_Re_v5_C2_z	-578.44247378	33.34	
125	2-Cuboctaedru_Re_v4_C2_t	-578.44247375	33.34	
126	3-Anticuboh_Re_v5_C2_h	-578.44163811	33.87	C-C
127	3-Anticuboh_Re_v5_C2_g	-578.44019066	34.77	
128	3-Anticuboh_Re_v4_C2_d_imag	-578.43994682	34.93	
129	3-Anticuboh_Re_v5_C2_m	-578.43513689	37.94	C-C
130	3-Anticuboh_Re_v6_C2_l	-578.43174699	40.07	
131	3-Anticuboh_Re_v4_C2_a_r-276	-578.43174691	40.07	C-C
132	3-Anticuboh_Re_v5_C2_b	-578.42678765	43.18	
133	3-Anticuboh_Re_v4_C2_g	-578.41549576	50.27	
134	3-Anticuboh_Re_v6_C2_k_imag	-578.41549576	50.27	
135	3-Anticuboh_Re_v5_C2_za	-578.40836728	54.74	C-C
136	3-Anticuboh_Re_v6_C2_o	-578.40707078	55.56	C-C
137	3-Anticuboh_Re_v4_C2_a_imag	-578.40589601	56.29	C-C
138	3-Anticuboh_Re_v6_C2_d	-578.39769827	61.44	C-C
139	3-Anticuboh_Re_v4_C2_r	-578.35034234	91.15	C-C
140	3-Anticuboh_Re_v5_C2_zd	-578.33620709	100.02	C-C

ω