

Neutral Rhenadiboranes with $\text{Re}(\text{CO})_2(\text{NO})$ Vertices: A Theoretical Study of Building Blocks for Rhenacarborane-based Drug Delivery Agents

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Supporting Information

Complete Gaussian09 Reference (reference 18).

Tables S1A-S1C. Initial models, distance matrices and energy rankings for the $\text{C}_2\text{B}_5\text{H}_7\text{Re}(\text{CO})_2\text{NO}$ structures

Tables S2A-S2C. Initial models, distance matrices and energy rankings for the $\text{C}_2\text{B}_6\text{H}_8\text{Re}(\text{CO})_2\text{NO}$ structures

Tables S3A-S3C. Initial models, distance matrices and energy rankings for the $\text{C}_2\text{B}_7\text{H}_9\text{Re}(\text{CO})_2\text{NO}$ structures

Tables S4A-S4C. Initial models, distance matrices and energy rankings for the $\text{C}_2\text{B}_8\text{H}_{10}\text{Re}(\text{CO})_2\text{NO}$ structures

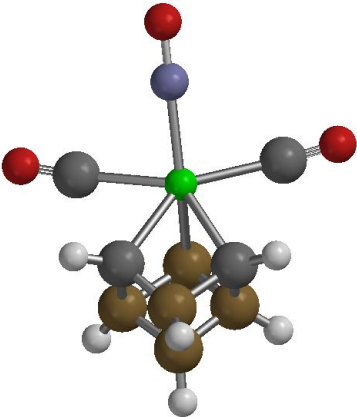
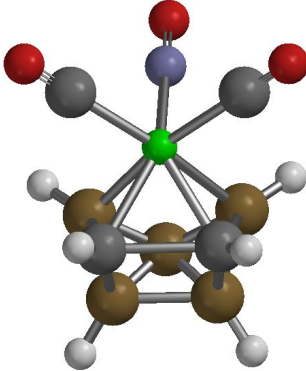
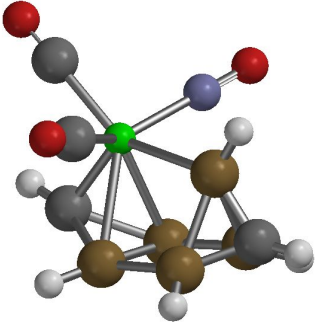
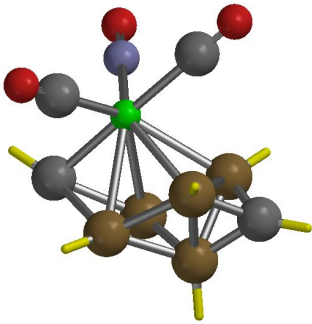
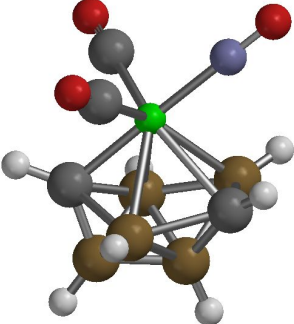
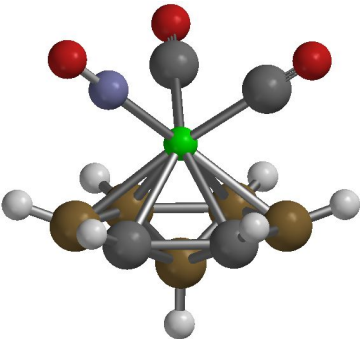
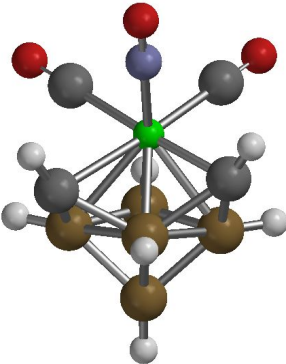
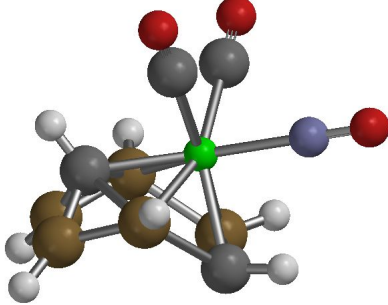
Tables S5A-S5C. Initial models, distance matrices and energy rankings for the $\text{C}_2\text{B}_9\text{H}_{11}\text{Re}(\text{CO})_2\text{NO}$ structures

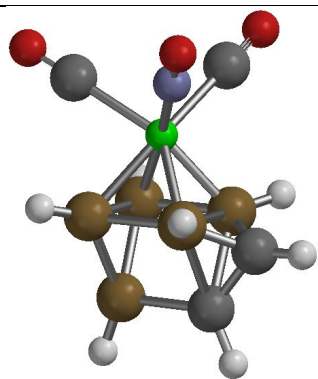
Table S6. Orbital energies and HOMO-LUMO gaps.

Complete Gaussian09 Reference.

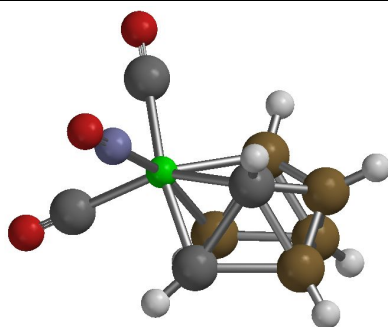
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Table 1A. Initial $(\text{CO})_2(\text{NO})\text{ReC}_2\text{B}_5\text{H}_7$ structures (one example from each family), a total of 414 structures:

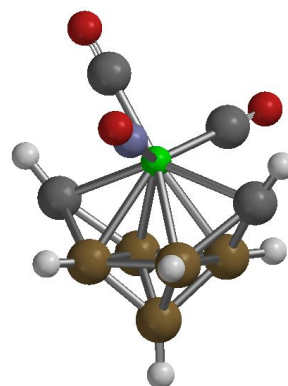
Initial structures	 1. Cube 18	 2. Antiprism 18
 3. Trigonal Prism 30	 4. Trigonal Antiprism 30	 5. Bisdisphenoid 54
 6. Hexagonal bipyramid 18	 7. All-capped tetrahedron 24	 8. Nido structure 24



9. Dicapped trigonal prism
(C_s) 78

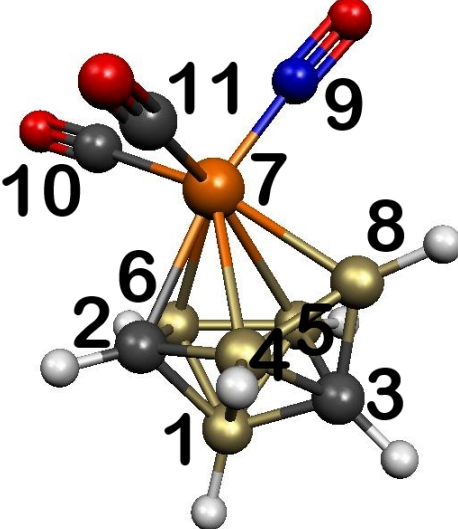
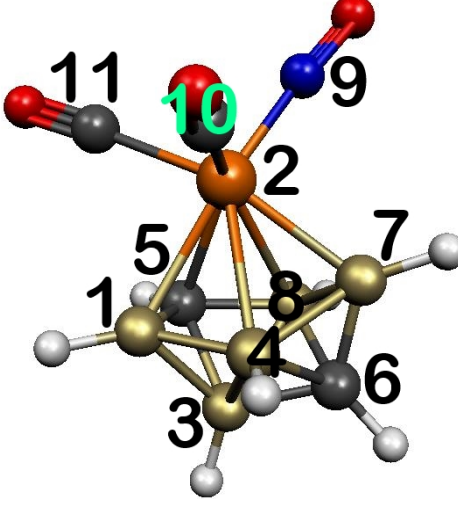


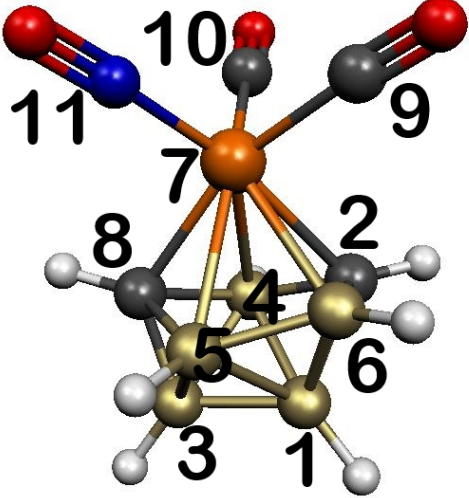
10. Dicapped trigonal prism
(C_{2v}) 60

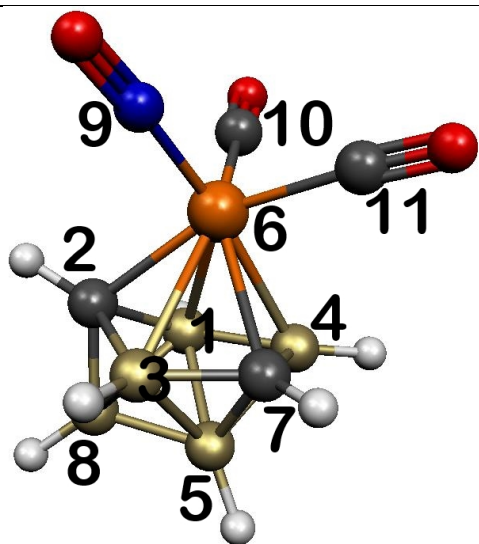


11. Dicapped octahedron 60

Table 1B. Distances table for the lowest-lying (CO)₂(NO)ReC₂B₅H₇ structures after M06L/6-311G(d,p)//SDD optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

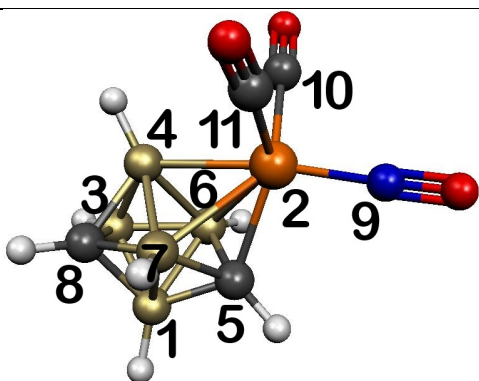
 1. -639.7933868 0.0 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>1.662868</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>1.579571</td><td>2.596306</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.862540</td><td>1.607041</td><td>1.676319</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.843895</td><td>2.522485</td><td>1.687585</td><td>2.507566</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.764105</td><td>1.554551</td><td>2.732890</td><td>2.628332</td><td>1.708130</td></tr><tr><td>7 Re</td><td>3.153242</td><td>2.229384</td><td>3.112291</td><td>2.400846</td><td>2.465428</td></tr><tr><td>8 B</td><td>2.642697</td><td>2.861645</td><td>1.504509</td><td>1.839810</td><td>1.855438</td></tr><tr><td>9 N</td><td>4.658683</td><td>4.036178</td><td>4.178545</td><td>3.886854</td><td>3.369701</td></tr><tr><td>10 C</td><td>4.215713</td><td>3.007260</td><td>4.758328</td><td>4.009969</td><td>3.694294</td></tr><tr><td>11 C</td><td>4.429144</td><td>3.096906</td><td>4.351054</td><td>3.007762</td><td>4.280193</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>2.294307</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.977610</td><td>2.211991</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 N</td><td>3.763752</td><td>1.833465</td><td>2.848197</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>2.674165</td><td>2.025590</td><td>4.150087</td><td>2.900759</td><td>0.000000</td></tr><tr><td>11 C</td><td>3.912823</td><td>1.988705</td><td>3.415013</td><td>2.850481</td><td>2.912291</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 C	1.662868	0.000000				3 C	1.579571	2.596306	0.000000			4 B	1.862540	1.607041	1.676319	0.000000		5 B	1.843895	2.522485	1.687585	2.507566	0.000000	6 B	1.764105	1.554551	2.732890	2.628332	1.708130	7 Re	3.153242	2.229384	3.112291	2.400846	2.465428	8 B	2.642697	2.861645	1.504509	1.839810	1.855438	9 N	4.658683	4.036178	4.178545	3.886854	3.369701	10 C	4.215713	3.007260	4.758328	4.009969	3.694294	11 C	4.429144	3.096906	4.351054	3.007762	4.280193		6	7	8	9	10	6 B	0.000000					7 Re	2.294307	0.000000				8 B	2.977610	2.211991	0.000000			9 N	3.763752	1.833465	2.848197	0.000000		10 C	2.674165	2.025590	4.150087	2.900759	0.000000	11 C	3.912823	1.988705	3.415013	2.850481	2.912291
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2. -639.7864854 +4.3 C₁	10 C 3.235520 1.975203 4.444218 2.984773 3.931672 11 C 2.882940 2.026454 4.234208 3.942755 2.813511 6 7 8 9 10 6 C 0.000000 7 B 1.503642 0.000000 8 B 1.675185 1.873716 0.000000 9 N 4.211207 2.941715 3.303419 0.000000 10 C 4.245209 3.201514 4.182454 2.815561 0.000000 11 C 4.785339 4.191950 3.802279 2.938269 2.893907
 3. -639.7818707 +7.2 C₁	1 2 3 4 5 1 B 0.000000 2 C 1.666707 0.000000 3 B 1.674141 2.740979 0.000000 4 B 1.865514 1.603793 1.794258 0.000000 5 B 1.918630 2.519965 1.823176 2.485724 0.000000 6 B 1.783711 1.547802 2.877096 2.617789 1.721329 7 Re 3.174765 2.227064 3.291670 2.410841 2.396656 8 C 2.492710 2.695548 1.506311 1.698391 1.690879 9 C 4.279281 3.009059 4.972813 3.998520 3.733781 10 C 4.459243 3.149764 4.469647 3.000254 4.199199 11 N 4.693261 4.034710 4.382748 3.950541 3.281767 6 7 8 9 10 6 B 0.000000 7 Re 2.271702 0.000000 8 C 2.818945 2.165021 0.000000 9 C 2.745983 2.008025 4.096619 0.000000 10 C 3.939388 1.991417 3.325465 2.877790 0.000000 11 N 3.703543 1.834874 2.984288 2.812614 2.845048



4. -639.7758567 +11.0 C₁

	1	2	3	4	5
1 B	0.000000				
2 C	1.682887	0.000000			
3 B	2.483510	1.709424	0.000000		
4 B	1.723115	2.826828	2.617249	0.000000	
5 B	1.914551	2.493823	1.873074	1.777295	0.000000
6 Re	2.400973	2.170123	2.407454	2.299700	3.188320
7 C	2.509908	2.697121	1.598915	1.541161	1.674550
8 B	1.825962	1.504922	1.802480	2.879380	1.673557
9 N	3.949024	3.003740	3.310373	4.121193	4.704523
10 C	2.940278	3.252961	4.168150	3.192694	4.464027
11 C	3.967107	4.116443	3.803130	2.972744	4.317002
	6	7	8	9	10
6 Re	0.000000				
7 C	2.228816	0.000000			
8 B	3.298654	2.742135	0.000000		
9 N	1.843054	3.676466	4.391875	0.000000	
10 C	1.972619	3.897413	4.426757	2.816874	0.000000
11 C	2.006175	2.864416	5.001228	2.844715	2.835205



5. -639.7717321 +13.6 C₁

	1	2	3	4	5
1 B	0.000000				
2 Re	3.334754	0.000000			
3 B	1.779317	3.563515	0.000000		
4 B	2.487402	2.296187	1.775147	0.000000	
5 C	1.600117	2.083570	2.734113	2.518806	0.000000
6 B	1.854252	2.393255	1.691891	1.921475	1.676875
7 B	1.835134	2.380470	2.614615	1.896842	1.661050
8 C	1.654887	3.431570	1.523603	1.665201	2.587838
9 N	4.616720	1.851510	5.197108	4.133926	3.050258
10 C	4.668976	1.971532	4.162318	2.906215	3.728206

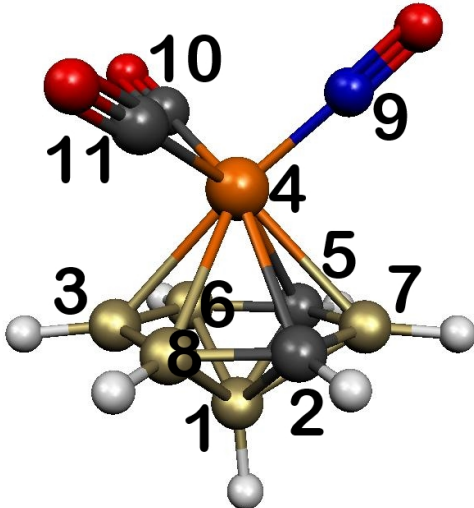
	11 C 4.652035 1.963185 4.754363 3.061401 3.651762					
	6 7 8 9 10					
	6 B 0.000000					
	7 B 2.477772 0.000000					
	8 C 2.471624 1.599108 0.000000					
	9 N 3.734513 3.816396 5.103824 0.000000					
	10 C 3.128156 3.996790 4.505449 2.893042 0.000000					
	11 C 4.092490 3.059469 4.147241 2.859780 2.756876					
6. -639.7494726 +27.6 C_s	1 2 3 4 5					
	1 B 0.000000					
	2 C 1.793564 0.000000					
	3 B 1.868487 2.679580 0.000000					
	4 Re 2.778705 2.333890 2.366865 0.000000					
	5 C 1.794398 2.552089 2.679190 2.334837 0.000000					
	6 B 1.876632 3.096621 1.646715 2.410060 1.529465					
	7 B 1.921961 1.530791 3.200534 2.395833 1.530410					
	8 B 1.875795 1.530026 1.646773 2.408833 3.096574					
	9 N 4.230703 3.323241 4.205103 1.846175 3.323826					
	10 C 4.069501 4.219893 3.051107 1.978398 3.254704					
	11 C 4.072773 3.256134 3.057112 1.978168 4.222067					
	6 7 8 9 10					
	6 B 0.000000					
	7 B 2.760852 0.000000					
	8 B 2.840337 2.761398 0.000000					
9 N 3.956453 2.985325 3.955926 0.000000						
10 C 2.706483 4.028092 3.918117 2.847725 0.000000						
11 C 3.922723 4.029008 2.710315 2.843523 2.828640						

Table 1C. Energy ranking for (CO)₂(NO)ReC₂B₅H₇ obtained after B3LYP/6-31G(d)//SDD optimization:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	02-Antipr---ReC2---20	-639.6086841	0.00
2	10-DicapTrPr-C2v---ReC2---328	-639.6086835	0.00
3	07-Tdallcap---ReC2---181	-639.6086695	0.01
4	07-Tdallcap---ReC2---192	-639.6086695	0.01
5	11-DicapOh---ReC2---400	-639.6086692	0.01
6	11-DicapOh---ReC2---411	-639.6086692	0.01
7	10-DicapTrPr-C2v---ReC2---302	-639.6086691	0.01
8	10-DicapTrPr-C2v---ReC2---333	-639.6086680	0.01
9	11-DicapOh---ReC2---374	-639.6086680	0.01
10	07-Tdallcap---ReC2---169	-639.6086678	0.01
11	10-DicapTrPr-C2v---ReC2---314	-639.6086678	0.01
12	04-AntiprTrig---ReC2---92	-639.6086671	0.01
13	08-Nido---ReC2---202	-639.6086671	0.01
14	10-DicapTrPr-C2v---ReC2---332	-639.6086629	0.01
15	11-DicapOh---ReC2---368	-639.6086606	0.01
16	11-DicapOh---ReC2---412	-639.6086597	0.02
17	05-Bisdisph---ReC2---138	-639.6086553	0.02
18	10-DicapTrPr-C2v---ReC2---306	-639.6086530	0.02
19	10-DicapTrPr-C2v---ReC2---308	-639.6086530	0.02
20	10-DicapTrPr-C2v---ReC2---346	-639.6086493	0.02
21	06-Bipirhex---ReC2---165	-639.6086481	0.02
22	06-Bipirhex---ReC2---158	-639.6086480	0.02
23	11-DicapOh---ReC2---394	-639.6086461	0.02
24	01-Cub---ReC2---11	-639.6086458	0.02
25	11-DicapOh---ReC2---399	-639.6086445	0.02
26	10-DicapTrPr-C2v---ReC2---350	-639.6086407	0.03

27	07-Tdallcap---ReC2---170	-639.6086403	0.03
28	04-AntiprTrig---ReC2---76	-639.6086392	0.03
29	01-Cub---ReC2---15	-639.6086384	0.03
30	10-DicapTrPr-C2v---ReC2---304	-639.6086358	0.03
31	05-Bisdisph---ReC2---148	-639.6086303	0.03
32	02-Antipr---ReC2---33	-639.6086223	0.04
33	05-Bisdisph---ReC2---109	-639.6086197	0.04
34	05-Bisdisph---ReC2---122	-639.6086197	0.04
35	09-DicapTrPr-Cs---ReC2---232	-639.6086176	0.04
36	11-DicapOh---ReC2---362	-639.6086163	0.04
37	10-DicapTrPr-C2v---ReC2---298	-639.6086004	0.05
38	11-DicapOh---ReC2---387	-639.6083232	0.23
39	05-Bisdisph---ReC2---106	-639.6083119	0.23
40	05-Bisdisph---ReC2---119	-639.6083030	0.24
41	01-Cub---ReC2---18	-639.6082997	0.24
42	01-Cub---ReC2---5	-639.6082997	0.24
43	05-Bisdisph---ReC2---120	-639.6082887	0.25
44	05-Bisdisph---ReC2---98	-639.6082887	0.25
45	08-Nido---ReC2---210	-639.6082880	0.25
46	09-DicapTrPr-Cs---ReC2---289	-639.6082863	0.25
47	01-Cub---ReC2---9	-639.6082853	0.25
48	10-DicapTrPr-C2v---ReC2---319	-639.6082790	0.25
49	09-DicapTrPr-Cs---ReC2---287	-639.6082666	0.26
50	10-DicapTrPr-C2v---ReC2---307	-639.6082663	0.26
51	09-DicapTrPr-Cs---ReC2---272	-639.6082650	0.26
52	09-DicapTrPr-Cs---ReC2---221	-639.6082644	0.26
53	09-DicapTrPr-Cs---ReC2---266	-639.6063620	1.46
54	09-DicapTrPr-Cs---ReC2---285	-639.6063620	1.46

55	08-Nido---ReC2---216	-639.6063606	1.46
56	08-Nido---ReC2---200	-639.6063585	1.46
57	04-AntiprTrig---ReC2---75	-639.6063558	1.46
58	04-AntiprTrig---ReC2---82	-639.6063558	1.46
59	04-AntiprTrig---ReC2---85	-639.6063526	1.46
60	06-Bipirhex---ReC2---153	-639.6063455	1.47
61	05-Bisdisph---ReC2---144	-639.6063449	1.47
62	10-DicapTrPr-C2v---ReC2---340	-639.6032211	3.43
63	09-DicapTrPr-Cs---ReC2---226	-639.6032120	3.43
64	09-DicapTrPr-Cs---ReC2---231	-639.6032120	3.43
65	10-DicapTrPr-C2v---ReC2---353	-639.6031834	3.45
66	11-DicapOh---ReC2---402	-639.6031819	3.45
67	05-Bisdisph---ReC2---105	-639.6031817	3.45
68	05-Bisdisph---ReC2---111	-639.6031817	3.45
69	05-Bisdisph---ReC2---112	-639.6031720	3.46
70	04-AntiprTrig---ReC2---77	-639.6031676	3.46
71	04-AntiprTrig---ReC2---95	-639.6031676	3.46
72	11-DicapOh---ReC2---392	-639.6031572	3.47
73	02-Antipr---ReC2---36	-639.6031042	3.50
74	02-Antipr---ReC2---24	-639.5960724	7.91
75	10-DicapTrPr-C2v---ReC2---339	-639.5960696	7.92
76	01-Cub---ReC2---12	-639.5960508	7.93
77	01-Cub---ReC2---1	-639.5960508	7.93
78	10-DicapTrPr-C2v---ReC2---347	-639.5960327	7.94
79	09-DicapTrPr-Cs---ReC2---224	-639.5960325	7.94
80	10-DicapTrPr-C2v---ReC2---320	-639.5960316	7.94
81	05-Bisdisph---ReC2---129	-639.5960245	7.94
82	07-Tdallcap---ReC2---171	-639.5960238	7.94

83	10-DicapTrPr-C2v---ReC2---295	-639.5960222	7.95
84	09-DicapTrPr-Cs---ReC2---273	-639.5960115	7.95
85	09-DicapTrPr-Cs---ReC2---293	-639.5960115	7.95
86	08-Nido---ReC2---194	-639.5960079	7.95
87	04-AntiprTrig---ReC2---72	-639.5960013	7.96
88	04-AntiprTrig---ReC2---96	-639.5960013	7.96
89	05-Bisdisph---ReC2---126	-639.5953245	8.38
90	05-Bisdisph---ReC2---97	-639.5953245	8.38
91	11-DicapOh---ReC2---397	-639.5953194	8.39
92	09-DicapTrPr-Cs---ReC2---219	-639.5953041	8.40
93	06-Bipirhex---ReC2---168	-639.5952952	8.40
94	10-DicapTrPr-C2v---ReC2---348	-639.5952943	8.40
95	05-Bisdisph---ReC2---125	-639.5952925	8.40
96	05-Bisdisph---ReC2---127	-639.5952792	8.41
97	05-Bisdisph---ReC2---133	-639.5952792	8.41
98	08-Nido---ReC2---208	-639.5952784	8.41
99	11-DicapOh---ReC2---404	-639.5906128	11.34
100	10-DicapTrPr-C2v---ReC2---341	-639.5906120	11.34
101	09-DicapTrPr-Cs---ReC2---217	-639.5906064	11.34
102	08-Nido---ReC2---206	-639.5905894	11.35
103	05-Bisdisph---ReC2---107	-639.5905834	11.36
104	06-Bipirhex---ReC2---164	-639.5905822	11.36
105	04-AntiprTrig---ReC2---74	-639.5905704	11.37
106	08-Nido---ReC2---213	-639.5902934	11.54
107	09-DicapTrPr-Cs---ReC2---267	-639.5902727	11.55
108	09-DicapTrPr-Cs---ReC2---291	-639.5902727	11.55
109	09-DicapTrPr-Cs---ReC2---228	-639.5902438	11.57
110	05-Bisdisph---ReC2---130	-639.5902432	11.57

111	05-Bisdisph---ReC2---139	-639.5902432	11.57
112	03-PrTrig---ReC2---41	-639.5902430	11.57
113	05-Bisdisph---ReC2---101	-639.5902150	11.59
114	09-DicapTrPr-Cs---ReC2---270	-639.5824022	16.49
115	09-DicapTrPr-Cs---ReC2---280	-639.5824022	16.49
116	11-DicapOh---ReC2---410	-639.5823954	16.50
117	08-Nido---ReC2---193	-639.5823940	16.50
118	08-Nido---ReC2---212	-639.5823940	16.50
119	05-Bisdisph---ReC2---141	-639.5823574	16.52
120	02-Antipr---ReC2---28	-639.5819236	16.79
121	10-DicapTrPr-C2v---ReC2---297	-639.5819088	16.80
122	10-DicapTrPr-C2v---ReC2---317	-639.5819079	16.80
123	11-DicapOh---ReC2---409	-639.5818982	16.81
124	10-DicapTrPr-C2v---ReC2---323	-639.5818772	16.82
125	10-DicapTrPr-C2v---ReC2---329	-639.5818772	16.82
126	06-Bipirhex---ReC2---152	-639.5818751	16.82
127	05-Bisdisph---ReC2---137	-639.5818659	16.83
128	05-Bisdisph---ReC2---146	-639.5818659	16.83
129	02-Antipr---ReC2---22	-639.5818531	16.84
130	02-Antipr---ReC2---26	-639.5818531	16.84
131	01-Cub---ReC2---3	-639.5786855	18.82
132	09-DicapTrPr-Cs---ReC2---281	-639.5786811	18.83
133	07-Tdallcap---ReC2---191	-639.5786670	18.84
134	11-DicapOh---ReC2---383	-639.5786632	18.84
135	11-DicapOh---ReC2---377	-639.5786550	18.84
136	09-DicapTrPr-Cs---ReC2---248	-639.5786268	18.86
137	04-AntiprTrig---ReC2---70	-639.5786062	18.87
138	11-DicapOh---ReC2---378	-639.5786007	18.88

139	11-DicapOh---ReC2---384	-639.5786007	18.88
140	03-PrTrig---ReC2---38	-639.5785965	18.88
141	11-DicapOh---ReC2---403	-639.5785869	18.89
142	08-Nido---ReC2---195	-639.5785824	18.89
143	08-Nido---ReC2---196	-639.5785794	18.89
144	08-Nido---ReC2---207	-639.5785794	18.89
145	07-Tdallcap---ReC2---186	-639.5785725	18.90
146	09-DicapTrPr-Cs---ReC2---282	-639.5785631	18.90
147	09-DicapTrPr-Cs---ReC2---276	-639.5785564	18.91
148	07-Tdallcap---ReC2---184	-639.5785560	18.91
149	07-Tdallcap---ReC2---189	-639.5785543	18.91
150	04-AntiprTrig---ReC2---67	-639.5762471	20.35
151	04-AntiprTrig---ReC2---90	-639.5762471	20.35
152	11-DicapOh---ReC2---386	-639.5762400	20.36
153	06-Bipirhex---ReC2---161	-639.5762396	20.36
154	09-DicapTrPr-Cs---ReC2---275	-639.5761900	20.39
155	09-DicapTrPr-Cs---ReC2---249	-639.5742527	21.61
156	04-AntiprTrig---ReC2---80	-639.5733369	22.18
157	03-PrTrig---ReC2---49	-639.5733247	22.19
158	11-DicapOh---ReC2---381	-639.5732889	22.21
159	09-DicapTrPr-Cs---ReC2---225	-639.5728677	22.48
160	05-Bisdisph---ReC2---135	-639.5728634	22.48
161	09-DicapTrPr-Cs---ReC2---279	-639.5728591	22.48
162	09-DicapTrPr-Cs---ReC2---294	-639.5728591	22.48
163	10-DicapTrPr-C2v---ReC2---337	-639.5728586	22.48
164	10-DicapTrPr-C2v---ReC2---345	-639.5728586	22.48
165	11-DicapOh---ReC2---401	-639.5728454	22.49
166	11-DicapOh---ReC2---405	-639.5728454	22.49

167	02-Antipr---ReC2---23	-639.5728442	22.49
168	05-Bisdisph---ReC2---136	-639.5728429	22.49
169	05-Bisdisph---ReC2---140	-639.5728429	22.49
170	10-DicapTrPr-C2v---ReC2---299	-639.5728373	22.49
171	10-DicapTrPr-C2v---ReC2---301	-639.5728243	22.50
172	10-DicapTrPr-C2v---ReC2---342	-639.5724829	22.72
173	11-DicapOh---ReC2---398	-639.5724767	22.72
174	08-Nido---ReC2---205	-639.5724630	22.73
175	08-Nido---ReC2---214	-639.5724630	22.73
176	09-DicapTrPr-Cs---ReC2---222	-639.5724496	22.74
177	11-DicapOh---ReC2---388	-639.5724483	22.74
178	03-PrTrig---ReC2---48	-639.5724438	22.74
179	03-PrTrig---ReC2---40	-639.5724418	22.74
180	09-DicapTrPr-Cs---ReC2---269	-639.5724411	22.74
181	09-DicapTrPr-Cs---ReC2---274	-639.5724411	22.74
182	10-DicapTrPr-C2v---ReC2---324	-639.5724048	22.77
183	05-Bisdisph---ReC2---102	-639.5715084	23.33
184	11-DicapOh---ReC2---373	-639.5713124	23.45
185	11-DicapOh---ReC2---389	-639.5713124	23.45
186	10-DicapTrPr-C2v---ReC2---327	-639.5659984	26.79
187	10-DicapTrPr-C2v---ReC2---334	-639.5659984	26.79
188	02-Antipr---ReC2---25	-639.5659947	26.79
189	02-Antipr---ReC2---34	-639.5659947	26.79
190	02-Antipr---ReC2---27	-639.5659903	26.79
191	06-Bipirhex---ReC2---167	-639.5659892	26.79
192	10-DicapTrPr-C2v---ReC2---315	-639.5659852	26.79
193	11-DicapOh---ReC2---414	-639.5659768	26.80
194	05-Bisdisph---ReC2---150	-639.5659759	26.80

195	10-DicapTrPr-C2v---ReC2---325	-639.5659731	26.80
196	09-DicapTrPr-Cs---ReC2---239	-639.5638904	28.11
197	09-DicapTrPr-Cs---ReC2---263	-639.5638904	28.11
198	07-Tdallcap---ReC2---182	-639.5625954	28.92
199	09-DicapTrPr-Cs---ReC2---254	-639.5625887	28.93
200	07-Tdallcap---ReC2---187	-639.5625880	28.93
201	02-Antipr---ReC2---35	-639.5625613	28.94
202	01-Cub---ReC2---8	-639.5625604	28.94
203	09-DicapTrPr-Cs---ReC2---271	-639.5625476	28.95
204	09-DicapTrPr-Cs---ReC2---284	-639.5625465	28.95
205	09-DicapTrPr-Cs---ReC2---290	-639.5625465	28.95
206	05-Bisdisph---ReC2---121	-639.5625440	28.95
207	07-Tdallcap---ReC2---180	-639.5625439	28.95
208	07-Tdallcap---ReC2---185	-639.5625434	28.95
209	05-Bisdisph---ReC2---115	-639.5625433	28.95
210	11-DicapOh---ReC2---407	-639.5625081	28.98
211	11-DicapOh---ReC2---413	-639.5625081	28.98
212	04-AntiprTrig---ReC2---87	-639.5610890	29.87
213	10-DicapTrPr-C2v---ReC2---338	-639.5610571	29.89
214	10-DicapTrPr-C2v---ReC2---351	-639.5610571	29.89
215	01-Cub---ReC2---7	-639.5610327	29.90
216	08-Nido---ReC2---203	-639.5610317	29.90
217	08-Nido---ReC2---209	-639.5610317	29.90
218	09-DicapTrPr-Cs---ReC2---234	-639.5610022	29.92
219	02-Antipr---ReC2---19	-639.5598803	30.63
220	02-Antipr---ReC2---31	-639.5598803	30.63
221	05-Bisdisph---ReC2---134	-639.5598761	30.63
222	08-Nido---ReC2---198	-639.5598737	30.63

223	10-DicapTrPr-C2v---ReC2---343	-639.5598572	30.64
224	10-DicapTrPr-C2v---ReC2---349	-639.5598572	30.64
225	10-DicapTrPr-C2v---ReC2---303	-639.5598483	30.65
226	09-DicapTrPr-Cs---ReC2---278	-639.5598477	30.65
227	09-DicapTrPr-Cs---ReC2---288	-639.5598477	30.65
228	09-DicapTrPr-Cs---ReC2---277	-639.5598431	30.65
229	10-DicapTrPr-C2v---ReC2---312	-639.5598418	30.65
230	10-DicapTrPr-C2v---ReC2---300	-639.5598413	30.65
231	08-Nido---ReC2---197	-639.5598276	30.66
232	08-Nido---ReC2---201	-639.5598276	30.66
233	06-Bipirhex---ReC2---155	-639.5589710	31.20
234	11-DicapOh---ReC2---375	-639.5589628	31.20
235	11-DicapOh---ReC2---376	-639.5589361	31.22
236	11-DicapOh---ReC2---382	-639.5589241	31.23
237	09-DicapTrPr-Cs---ReC2---220	-639.5583408	31.59
238	09-DicapTrPr-Cs---ReC2---229	-639.5583408	31.59
239	10-DicapTrPr-C2v---ReC2---354	-639.5583239	31.60
240	09-DicapTrPr-Cs---ReC2---230	-639.5583212	31.60
241	05-Bisdisph---ReC2---114	-639.5583155	31.61
242	05-Bisdisph---ReC2---99	-639.5583155	31.61
243	05-Bisdisph---ReC2---113	-639.5583125	31.61
244	04-AntiprTrig---ReC2---73	-639.5582986	31.62
245	04-AntiprTrig---ReC2---88	-639.5582986	31.62
246	04-AntiprTrig---ReC2---79	-639.5577768	31.95
247	04-AntiprTrig---ReC2---86	-639.5577768	31.95
248	10-DicapTrPr-C2v---ReC2---311	-639.5577661	31.95
249	08-Nido---ReC2---199	-639.5577570	31.96
250	08-Nido---ReC2---215	-639.5577570	31.96

251	09-DicapTrPr-Cs---ReC2---265	-639.5577563	31.96
252	09-DicapTrPr-Cs---ReC2---227	-639.5577440	31.97
253	05-Bisdisph---ReC2---104	-639.5577432	31.97
254	05-Bisdisph---ReC2---117	-639.5577432	31.97
255	05-Bisdisph---ReC2---118	-639.5577211	31.98
256	09-DicapTrPr-Cs---ReC2---235	-639.5526149	35.18
257	09-DicapTrPr-Cs---ReC2---256	-639.5526149	35.18
258	09-DicapTrPr-Cs---ReC2---247	-639.5525967	35.20
259	09-DicapTrPr-Cs---ReC2---253	-639.5525967	35.20
260	09-DicapTrPr-Cs---ReC2---241	-639.5520859	35.52
261	09-DicapTrPr-Cs---ReC2---258	-639.5520395	35.55
262	05-Bisdisph---ReC2---124	-639.5520341	35.55
263	05-Bisdisph---ReC2---103	-639.5520234	35.56
264	05-Bisdisph---ReC2---123	-639.5520234	35.56
265	09-DicapTrPr-Cs---ReC2---261	-639.5514792	35.90
266	05-Bisdisph---ReC2---100	-639.5508780	36.27
267	05-Bisdisph---ReC2---108	-639.5508780	36.27
268	10-DicapTrPr-C2v---ReC2---296	-639.5501045	36.76
269	10-DicapTrPr-C2v---ReC2---305	-639.5501045	36.76
270	11-DicapOh---ReC2---406	-639.5500968	36.76
271	10-DicapTrPr-C2v---ReC2---352	-639.5499502	36.86
272	11-DicapOh---ReC2---363	-639.5499176	36.88
273	01-Cub---ReC2---2	-639.5499088	36.88
274	09-DicapTrPr-Cs---ReC2---283	-639.5485028	37.76
275	05-Bisdisph---ReC2---110	-639.5484722	37.78
276	05-Bisdisph---ReC2---116	-639.5484722	37.78
277	10-DicapTrPr-C2v---ReC2---330	-639.5484073	37.82
278	05-Bisdisph---ReC2---132	-639.5484059	37.83

279	09-DicapTrPr-Cs---ReC2---244	-639.5483736	37.85
280	10-DicapTrPr-C2v---ReC2---313	-639.5481382	37.99
281	10-DicapTrPr-C2v---ReC2---336	-639.5481182	38.01
282	02-Antipr---ReC2---30	-639.5481127	38.01
283	02-Antipr---ReC2---29	-639.5481080	38.01
284	05-Bisdisph---ReC2---131	-639.5480879	38.03
285	05-Bisdisph---ReC2---145	-639.5480879	38.03
286	09-DicapTrPr-Cs---ReC2---268	-639.5477111	38.26
287	10-DicapTrPr-C2v---ReC2---316	-639.5477087	38.26
288	10-DicapTrPr-C2v---ReC2---326	-639.5477082	38.26
289	10-DicapTrPr-C2v---ReC2---321	-639.5476967	38.27
290	10-DicapTrPr-C2v---ReC2---335	-639.5476967	38.27
291	05-Bisdisph---ReC2---143	-639.5476854	38.28
292	05-Bisdisph---ReC2---149	-639.5476854	38.28
293	08-Nido---ReC2---204	-639.5474897	38.40
294	11-DicapOh---ReC2---367	-639.5474594	38.42
295	09-DicapTrPr-Cs---ReC2---243_r-211	-639.5468776	38.78
296	02-Antipr---ReC2---21	-639.5468695	38.79
297	10-DicapTrPr-C2v---ReC2---344	-639.5468113	38.83
298	01-Cub---ReC2---10	-639.5463563	39.11
299	01-Cub---ReC2---13	-639.5463563	39.11
300	09-DicapTrPr-Cs---ReC2---233	-639.5462240	39.19
301	06-Bipirhex---ReC2---156	-639.5453751	39.73
302	06-Bipirhex---ReC2---151	-639.5453633	39.74
303	09-DicapTrPr-Cs---ReC2---243_i-211	-639.5452113	39.83
304	08-Nido---ReC2---211	-639.5440913	40.53
305	09-DicapTrPr-Cs---ReC2---218	-639.5440852	40.54
306	09-DicapTrPr-Cs---ReC2---223	-639.5440852	40.54

307	10-DicapTrPr-C2v---ReC2---331	-639.5432526	41.06
308	02-Antipr---ReC2---32	-639.5426748	41.42
309	04-AntiprTrig---ReC2---81	-639.5426675	41.43
310	10-DicapTrPr-C2v---ReC2---310	-639.5426557	41.43
311	10-DicapTrPr-C2v---ReC2---309	-639.5418945	41.91
312	10-DicapTrPr-C2v---ReC2---318	-639.5418922	41.91
313	05-Bisdisph---ReC2---147	-639.5418644	41.93
314	07-Tdallcap---ReC2---188	-639.5403109	42.91
315	03-PrTrig---ReC2---42	-639.5362880	45.43
316	03-PrTrig---ReC2---66	-639.5362880	45.43
317	09-DicapTrPr-Cs---ReC2---236	-639.5355257	45.91
318	09-DicapTrPr-Cs---ReC2---250	-639.5355257	45.91
319	07-Tdallcap---ReC2---190	-639.5348751	46.32
320	03-PrTrig---ReC2---56	-639.5347937	46.37
321	03-PrTrig---ReC2---52	-639.5347708	46.38
322	03-PrTrig---ReC2---57	-639.5347708	46.38
323	11-DicapOh---ReC2---372	-639.5347653	46.39
324	11-DicapOh---ReC2---359	-639.5347597	46.39
325	11-DicapOh---ReC2---371	-639.5347597	46.39
326	01-Cub---ReC2---4	-639.5338364	46.97
327	04-AntiprTrig---ReC2---94	-639.5332223	47.35
328	07-Tdallcap---ReC2---174	-639.5332126	47.36
329	07-Tdallcap---ReC2---183	-639.5332119	47.36
330	04-AntiprTrig---ReC2---68	-639.5300272	49.36
331	04-AntiprTrig---ReC2---71	-639.5294939	49.69
332	04-AntiprTrig---ReC2---78	-639.5294939	49.69
333	10-DicapTrPr-C2v---ReC2---322	-639.5285039	50.31
334	11-DicapOh---ReC2---408	-639.5268551	51.35

335	01-Cub---ReC2---6	-639.5254378	52.24
336	07-Tdallcap---ReC2---173	-639.5254199	52.25
337	04-AntiprTrig---ReC2---89	-639.5254145	52.25
338	04-AntiprTrig---ReC2---91	-639.5254145	52.25
339	05-Bisdisph---ReC2---142	-639.5253079	52.32
340	03-PrTrig---ReC2---61	-639.5194845	55.97
341	09-DicapTrPr-Cs---ReC2---246	-639.5166929	57.73
342	09-DicapTrPr-Cs---ReC2---264	-639.5166929	57.73
343	03-PrTrig---ReC2---37	-639.5157045	58.35
344	11-DicapOh---ReC2---361	-639.5154256	58.52
345	09-DicapTrPr-Cs---ReC2---257	-639.5152949	58.60
346	09-DicapTrPr-Cs---ReC2---259	-639.5152949	58.60
347	09-DicapTrPr-Cs---ReC2---262	-639.5152519	58.63
348	09-DicapTrPr-Cs---ReC2---251	-639.5141872	59.30
349	09-DicapTrPr-Cs---ReC2---260	-639.5141872	59.30
350	09-DicapTrPr-Cs---ReC2---242	-639.5132109	59.91
351	09-DicapTrPr-Cs---ReC2---252	-639.5132109	59.91
352	03-PrTrig---ReC2---59	-639.5130386	60.02
353	03-PrTrig---ReC2---65	-639.5130386	60.02
354	11-DicapOh---ReC2---357	-639.5123448	60.45
355	11-DicapOh---ReC2---360	-639.5122064	60.54
356	03-PrTrig---ReC2---62	-639.5108493	61.39
357	11-DicapOh---ReC2---369	-639.5108489	61.39
358	06-Bipirhex---ReC2---163	-639.5107590	61.45
359	05-Bisdisph---ReC2---128	-639.5107461	61.46
360	06-Bipirhex---ReC2---162	-639.5103929	61.68
361	06-Bipirhex---ReC2---166	-639.5103928	61.68
362	06-Bipirhex---ReC2---157	-639.5103545	61.70

363	03-PrTrig---ReC2---44	-639.5093014	62.36
364	11-DicapOh---ReC2---379	-639.5082270	63.04
365	11-DicapOh---ReC2---390	-639.5082270	63.04
366	09-DicapTrPr-Cs---ReC2---292	-639.5074078	63.55
367	09-DicapTrPr-Cs---ReC2---238	-639.5053759	64.83
368	07-Tdallcap---ReC2---176	-639.5048562	65.15
369	07-Tdallcap---ReC2---172	-639.5048462	65.16
370	07-Tdallcap---ReC2---177	-639.5048462	65.16
371	04-AntiprTrig---ReC2---83	-639.5048387	65.17
372	04-AntiprTrig---ReC2---93	-639.5048387	65.17
373	01-Cub---ReC2---17	-639.5048351	65.17
374	03-PrTrig---ReC2---53	-639.5035825	65.95
375	03-PrTrig---ReC2---63	-639.5035825	65.95
376	11-DicapOh---ReC2---364	-639.5035741	65.96
377	11-DicapOh---ReC2---370	-639.5035741	65.96
378	06-Bipirhex---ReC2---159	-639.5030267	66.30
379	03-PrTrig---ReC2---39	-639.5021792	66.83
380	03-PrTrig---ReC2---54	-639.5021792	66.83
381	04-AntiprTrig---ReC2---69	-639.5021775	66.84
382	04-AntiprTrig---ReC2---84	-639.5021775	66.84
383	01-Cub---ReC2---14	-639.5021448	66.86
384	09-DicapTrPr-Cs---ReC2---286	-639.5018662	67.03
385	11-DicapOh---ReC2---391	-639.5013939	67.33
386	11-DicapOh---ReC2---380	-639.5013720	67.34
387	11-DicapOh---ReC2---395	-639.5013720	67.34
388	11-DicapOh---ReC2---358	-639.5001805	68.09
389	11-DicapOh---ReC2---365	-639.5001805	68.09
390	07-Tdallcap---ReC2---178	-639.5000059	68.20

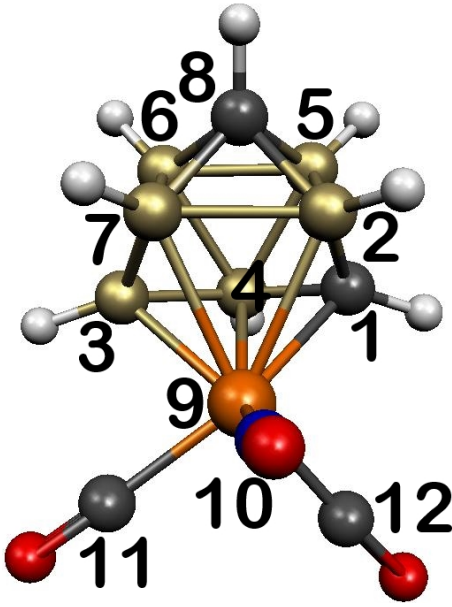
391	07-Tdallcap---ReC2---179	-639.4999283	68.25
392	09-DicapTrPr-Cs---ReC2---240	-639.4989436	68.86
393	09-DicapTrPr-Cs---ReC2---245	-639.4989436	68.86
394	03-PrTrig---ReC2---47	-639.4989023	68.89
395	03-PrTrig---ReC2---64	-639.4989023	68.89
396	06-Bipirhex---ReC2---154	-639.4979405	69.49
397	06-Bipirhex---ReC2---160	-639.4979405	69.49
398	11-DicapOh---ReC2---356	-639.4976477	69.68
399	03-PrTrig---ReC2---55	-639.4976404	69.68
400	09-DicapTrPr-Cs---ReC2---237	-639.4970863	70.03
401	01-Cub---ReC2---16	-639.4954722	71.04
402	11-DicapOh---ReC2---355	-639.4949305	71.38
403	11-DicapOh---ReC2---366	-639.4949262	71.39
404	03-PrTrig---ReC2---45	-639.4913457	73.63
405	03-PrTrig---ReC2---51	-639.4913457	73.63
406	03-PrTrig---ReC2---46	-639.4907272	74.02
407	03-PrTrig---ReC2---58	-639.4907272	74.02
408	07-Tdallcap---ReC2---175	-639.4906962	74.04
409	03-PrTrig---ReC2---60	-639.4900794	74.43
410	09-DicapTrPr-Cs---ReC2---255	-639.4884377	75.46
411	11-DicapOh---ReC2---393	-639.4805940	80.38
412	03-PrTrig---ReC2---50	-639.4689934	87.66
413	11-DicapOh---ReC2---385	-639.4430826	103.92
414	11-DicapOh---ReC2---396	-639.4430826	103.92
415	03-PrTrig---ReC2---43	-639.4426531	104.19

Table 2A. Initial $(\text{CO})_2(\text{NO})\text{ReC}_2\text{B}_6\text{H}_8$ structures (one example from each family), a total of 294 structures:

Initial structures
1. Capped cube 49 structures
2. Pressed capped cube 77 structures
3. $\text{Tl}_9^9\text{-like}$ structure 105 structures

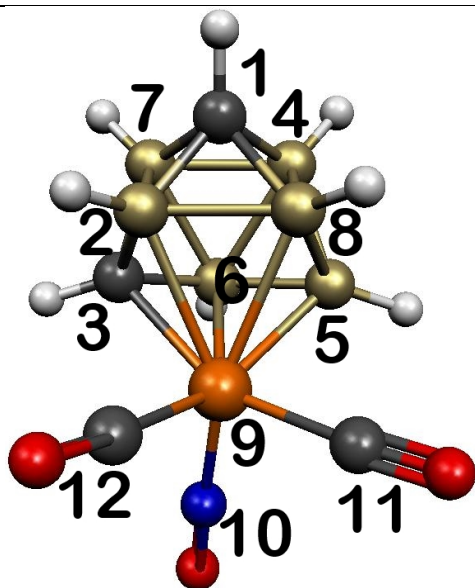
4. Tricapped trigonal prism 63 structures

Table 2B. Distances table for the lowest-lying (CO)₂(NO)ReC₂B₆H₈ structures after M06L/6-311G(d,p)//SDD optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.



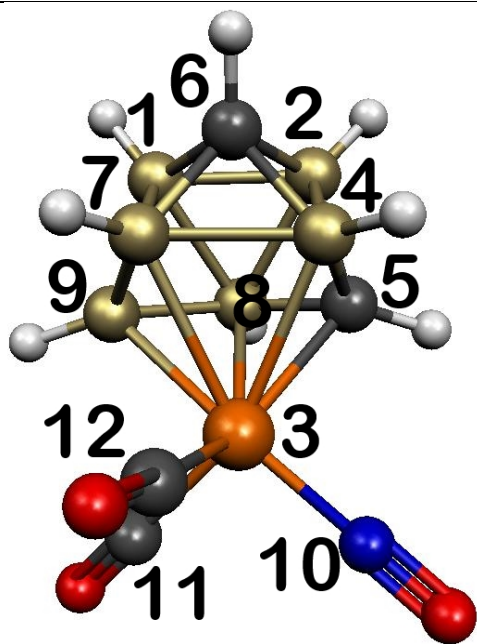
1. -665.2652111 0.0 C₁

	1	2	3	4	5
1 C	0.000000				
2 B	1.606510	0.000000			
3 B	2.799569	2.959078	0.000000		
4 B	1.611148	2.618407	1.751054	0.000000	
5 B	1.610930	1.792801	2.891095	1.893936	0.000000
6 B	2.745634	2.628913	1.697136	1.919718	1.861891
7 B	2.824806	1.995382	1.730235	2.659429	2.627637
8 C	2.557175	1.595226	2.708853	2.727654	1.584502
9 Re	2.159203	2.425438	2.205465	2.372767	3.307733
10 N	3.456295	2.991535	3.656792	4.105598	4.516741
11 C	3.952132	4.278308	2.583934	3.455690	4.899822
12 C	2.827558	3.756665	3.860297	3.312657	4.393324
	6	7	8	9	10
6 B	0.000000				
7 B	1.781243	0.000000			
8 C	1.602554	1.591045	0.000000		
9 Re	3.293521	2.447208	3.358028	0.000000	
10 N	4.586680	3.137886	4.126246	1.841724	0.000000
11 C	4.234546	3.478327	4.803002	1.992354	2.858668
12 C	4.879940	4.391109	4.978607	2.005854	2.888837
	11	12			
12 C	2.885432	0.000000			



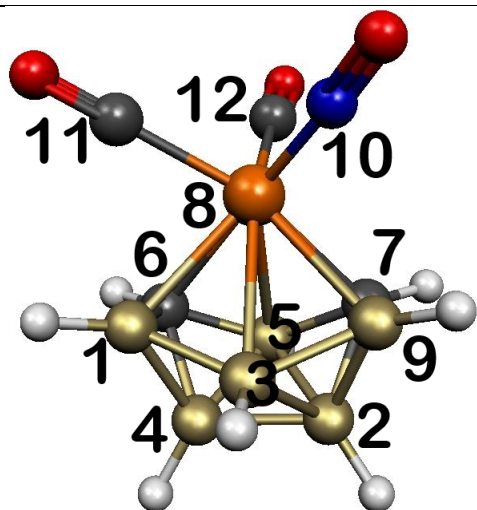
2. -665.2609054 +2.7 C₁

	1	2	3	4	5
1 C	0.000000				
2 B	1.598456	0.000000			
3 C	2.568295	1.632095	0.000000		
4 B	1.591596	2.617000	2.765820	0.000000	
5 B	2.724131	2.951991	2.813538	1.683016	0.000000
6 B	2.748762	2.620526	1.607122	1.964897	1.736347
7 B	1.582413	1.796541	1.594178	1.898788	2.898436
8 B	1.595220	1.913971	2.800340	1.783360	1.769968
9 Re	3.403337	2.448621	2.165614	3.294519	2.209873
10 N	5.070886	4.090231	3.207848	4.667302	3.365337
11 C	4.428008	3.852102	4.072996	4.182215	2.760159
12 C	4.299786	2.857404	3.092510	4.834190	4.088591
	6	7	8	9	10
6 B	0.000000				
7 B	1.923272	0.000000			
8 B	2.655242	2.612904	0.000000		
9 Re	2.310526	3.305969	2.452620	0.000000	
10 N	3.114521	4.587100	4.198428	1.833312	0.000000
11 C	3.840696	4.879526	2.932502	1.997776	2.824336
12 C	4.033374	4.345045	3.580609	2.022181	2.899708
	11	12			
12 C	2.911689	0.000000			



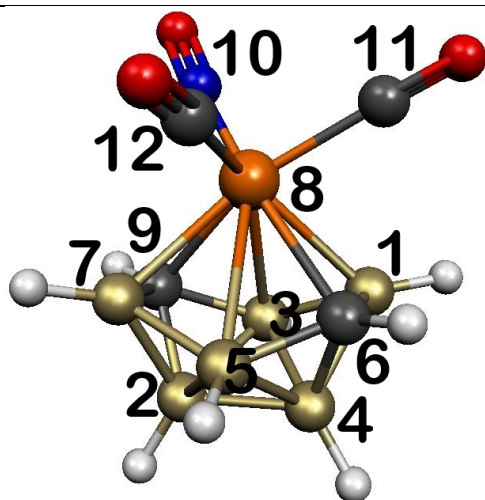
3. -665.2593055 +3.7 C₁

	1	2	3	4	5
1 B	0.000000				
2 B	1.875376	0.000000			
3 Re	3.311815	3.303404	0.000000		
4 B	2.643288	1.796093	2.428069	0.000000	
5 C	2.742085	1.599399	2.143796	1.617963	0.000000
6 C	1.608591	1.584962	3.371127	1.599931	2.553760
7 B	1.776246	2.627358	2.484614	2.002641	2.826972
8 B	1.927514	1.906159	2.363583	2.631138	1.602165
9 B	1.688757	2.899499	2.239462	2.967056	2.804212
10 N	4.974244	4.415275	1.855231	3.415068	2.877741
11 C	4.217756	4.750714	1.978789	4.302804	3.715832
12 C	4.398329	4.719803	1.983720	3.331320	3.852549
	6	7	8	9	10
6 C	0.000000				
7 B	1.586004	0.000000			
8 B	2.734130	2.662625	0.000000		
9 B	2.702444	1.719388	1.763672	0.000000	
10 N	4.790043	4.196009	3.655331	4.043748	0.000000
11 C	4.874555	3.709396	3.150334	2.617345	2.881422
12 C	4.140407	2.865455	4.138263	3.289340	2.832400
	11	12			
11 C	0.000000				
12 C	2.840498	0.000000			



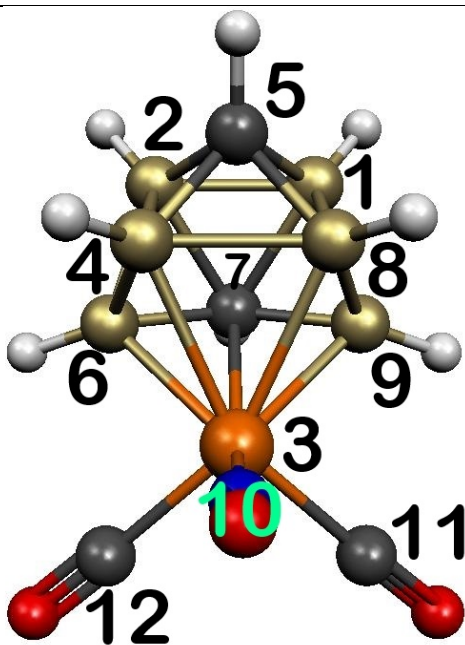
4. -665.2524353 +8.0 (Cs)

	1	2	3	4	5
1 B	0.000000				
2 B	2.887782	0.000000			
3 B	1.728528	1.835907	0.000000		
4 B	1.743943	1.736287	1.835083	0.000000	
5 B	2.698944	1.806797	2.735002	1.807111	0.000000
6 C	1.538428	2.746525	2.587321	1.658435	1.616428
7 C	3.292522	1.662259	2.590832	2.756047	1.628648
8 Re	2.305775	3.087779	2.495121	3.094228	2.573353
9 B	3.059001	1.738221	1.737776	2.888947	2.694941
10 N	3.776424	4.241431	3.470670	4.669848	4.197879
11 C	2.612492	4.765948	3.634312	4.134466	4.100893
12 C	3.901866	4.343096	4.353877	4.390381	3.129386
	6	7	8	9	10
6 C	0.000000				
7 C	2.771922	0.000000			
8 Re	2.249303	2.238242	0.000000		
9 B	3.287653	1.524546	2.297037	0.000000	
10 N	4.073514	3.239776	1.839058	2.755877	0.000000
11 C	2.973544	4.220971	2.022457	4.096280	2.743490
12 C	3.096135	2.992147	2.006154	3.809071	2.872436
	11	12			
11 C	0.000000				
12 C	2.910567	0.000000			



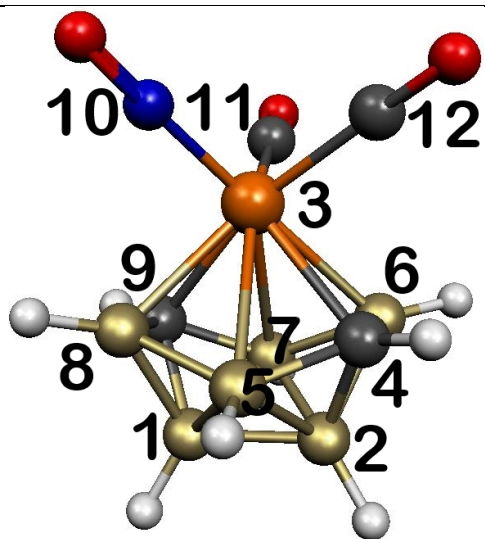
5. -665.2495105 +9.9 (C₂)

	1	2	3	4	5
1 B	0.000000				
2 B	2.900804	0.000000			
3 B	1.747508	1.840978	0.000000		
4 B	1.757072	1.737285	1.840539	0.000000	
5 B	2.705235	1.809371	2.746685	1.813615	0.000000
6 C	1.538615	2.733925	2.591326	1.647616	1.604864
7 B	3.427349	1.765933	2.698575	2.906284	1.764206
8 Re	2.273530	3.073650	2.451864	3.086620	2.601835
9 C	2.950425	1.638192	1.626312	2.757434	2.601485
10 N	3.698533	4.295417	3.426907	4.667867	4.280657
11 C	2.630351	4.775092	3.738144	4.115861	4.003095
12 C	3.921302	4.195758	4.262103	4.364482	3.064508
	6	7	8	9	10
6 C	0.000000				
7 B	2.904249	0.000000			
8 Re	2.277717	2.302565	0.000000		
9 C	3.168627	1.518994	2.218828	0.000000	
10 N	4.088867	3.348686	1.835257	2.852999	0.000000
11 C	2.877482	4.261863	2.027253	4.116432	2.776405
12 C	3.165986	2.778439	1.998078	3.590948	2.860234
	11	12			
11 C	0.000000				
12 C	2.883205	0.000000			



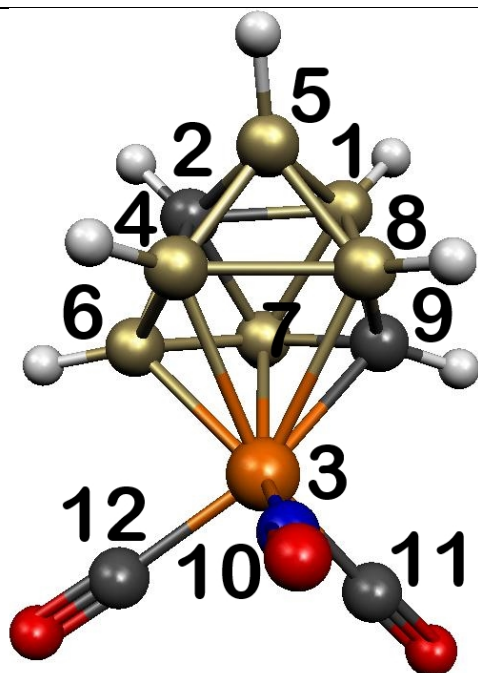
6. -665.2467502 +11.6 C_s

	1	2	3	4	5
1 B	0.000000				
2 B	1.849832	0.000000			
3 Re	3.287030	3.286922	0.000000		
4 B	2.620192	1.776175	2.441403	0.000000	
5 C	1.584541	1.584606	3.361079	1.597922	0.000000
6 B	2.860479	1.691805	2.195841	1.728483	2.699754
7 C	1.819661	1.818606	2.316973	2.531214	2.613346
8 B	1.776514	2.620453	2.442055	2.005961	1.597712
9 B	1.691391	2.859322	2.195457	2.958407	2.699311
10 N	4.544696	4.542908	1.829660	3.074549	4.141146
11 C	4.273261	4.864404	2.003321	4.345539	4.882819
12 C	4.864530	4.276097	2.003546	3.615000	4.886423
	6	7	8	9	10
6 B	0.000000				
7 C	1.642916	0.000000			
8 B	2.959604	2.532665	0.000000		
9 B	2.874600	1.643145	1.729480	0.000000	
10 N	3.573500	4.030213	3.077530	3.577013	0.000000
11 C	3.913462	3.351418	3.609740	2.630070	2.878976
12 C	2.633402	3.349002	4.347981	3.910148	2.878830
	11	12			
11 C	0.000000				
12 C	2.913876	0.000000			



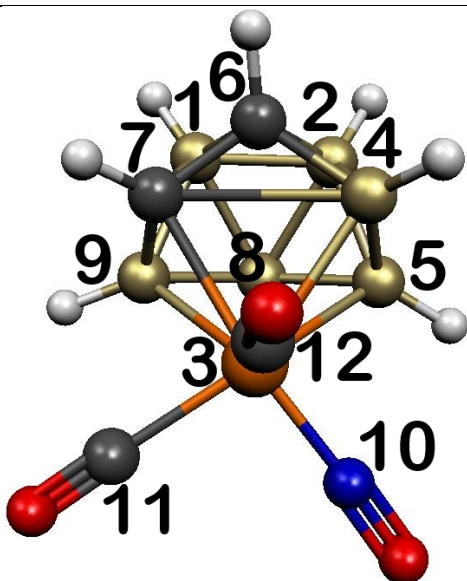
7. -665.2440586 +13.3 (C₂)

	1	2	3	4	5
1 B	0.000000				
2 B	1.734478	0.000000			
3 Re	3.085560	3.101448	0.000000		
4 C	2.748200	1.645179	2.257090	0.000000	
5 B	1.832956	1.834620	2.495408	1.614215	0.000000
6 B	2.896282	1.760864	2.326527	1.525845	2.694106
7 B	1.819928	1.816192	2.570702	2.592384	2.740842
8 B	1.749241	2.903182	2.277119	2.945191	1.761055
9 C	1.652861	2.754069	2.255746	3.176483	2.598988
10 N	4.270048	4.724836	1.845141	3.813125	3.564218
11 C	4.266292	4.283547	1.985652	3.777871	4.296586
12 C	4.782586	4.177094	2.019361	2.714534	3.656875
	6	7	8	9	10
6 B	0.000000				
7 B	1.746950	0.000000			
8 B	3.427822	2.695374	0.000000		
9 C	2.924199	1.624125	1.518136	0.000000	
10 N	4.167628	4.183490	2.775690	3.236133	0.000000
11 C	2.998527	3.001121	3.766645	2.956959	2.856585
12 C	2.974867	4.115008	4.086726	4.240406	2.753798
	11	12			
11 C	0.000000				
12 C	2.879871	0.000000			



8. -665.2363115 +18.1 C₁

	1	2	3	4	5
1 B	0.000000				
2 C	1.778187	0.000000			
3 Re	3.317060	3.147275	0.000000		
4 B	2.611806	1.690083	2.429827	0.000000	
5 B	1.676874	1.625435	3.521975	1.679185	0.000000
6 B	2.885467	1.612903	2.193252	1.729137	2.828746
7 B	1.884131	1.809784	2.361971	2.638030	2.860708
8 B	1.776669	2.491764	2.476084	1.977840	1.692329
9 C	1.606726	2.600542	2.170326	2.793971	2.696303
10 N	4.530010	4.440329	1.841953	3.110601	4.256293
11 C	4.397824	4.742790	2.006121	4.368524	5.137118
12 C	4.921102	4.161345	1.985587	3.514628	4.980740
	6	7	8	9	10
6 B	0.000000				
7 B	1.747391	0.000000			
8 B	2.970054	2.615043	0.000000		
9 C	2.791764	1.597950	1.612146	0.000000	
10 N	3.635797	4.092784	3.045466	3.470265	0.000000
11 C	3.869505	3.321098	3.781611	2.834100	2.875965
12 C	2.619592	3.466698	4.335633	3.961782	2.838549
	11	12			
11 C	0.000000				
12 C	2.868874	0.000000			



9. -665.2236182 +26.1 (C_2)

	1	2	3	4	5
1 B	0.000000				
2 B	1.779959	0.000000			
3 Re	3.205965	3.173981	0.000000		
4 B	2.798004	1.756702	2.401010	0.000000	
5 B	2.888237	1.692770	2.263847	1.659980	0.000000
6 C	1.666241	1.683038	2.910645	1.616873	2.652455
7 C	1.664929	2.659243	2.341357	2.542793	3.143276
8 B	1.843295	1.844787	2.449737	2.722317	1.758616
9 B	1.722615	2.869229	2.262305	3.263815	3.017892
10 N	4.755143	4.270411	1.829009	3.434957	2.748272
11 C	4.212346	4.841091	2.027206	4.338522	4.121277
12 C	4.395064	4.302502	1.989186	2.848884	3.633481
	6	7	8	9	10
6 C	0.000000				
7 C	1.518766	0.000000			
8 B	2.668210	2.559848	0.000000		
9 B	2.626241	1.564154	1.718581	0.000000	
10 N	4.474037	4.153334	3.444199	3.805347	0.000000
11 C	4.374367	3.161716	3.615375	2.618418	2.853042
12 C	3.406173	3.018306	4.231472	3.761142	2.889708
	11	12			
11 C	0.000000				
12 C	2.961786	0.000000			

Table 2C. Energy ranking for (CO)₂(NO)ReC₂B₆H₈ obtained after B3LYP/6-31G(d)//SDD optimization:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	01-CapCube---ReC2---7	-665.0680266	0.00
2	02-PressCapCube---ReC2---104	-665.0680076	0.01
3	02-PressCapCube---ReC2---81	-665.0680049	0.01
4	02-PressCapCube---ReC2---117	-665.0679898	0.02
5	03-Tl99---ReC2---181	-665.0679732	0.03
6	04-TrTrPr---ReC2---232	-665.0667938	0.77
7	04-TrTrPr---ReC2---246	-665.0667938	0.77
8	01-CapCube---ReC2---11	-665.0667851	0.78
9	02-PressCapCube---ReC2---103	-665.0667670	0.79
10	01-CapCube---ReC2---49	-665.0667654	0.79
11	01-CapCube---ReC2---20	-665.0667622	0.79
12	02-PressCapCube---ReC2---86	-665.0667113	0.83
13	02-PressCapCube---ReC2---95	-665.0624525	3.50
14	04-TrTrPr---ReC2---247	-665.0616402	4.01
15	02-PressCapCube---ReC2---82	-665.0616040	4.03
16	02-PressCapCube---ReC2---98	-665.0616040	4.03
17	03-Tl99---ReC2---195	-665.0558072	7.67
18	03-Tl99---ReC2---174	-665.0537095	8.98
19	03-Tl99---ReC2---196	-665.0537072	8.99
20	01-CapCube---ReC2---10	-665.0536961	8.99
21	04-TrTrPr---ReC2---233	-665.0536862	9.00
22	01-CapCube---ReC2---21	-665.0525907	9.69
23	03-Tl99---ReC2---224	-665.0490144	11.93
24	04-TrTrPr---ReC2---245	-665.0489678	11.96
25	04-TrTrPr---ReC2---259	-665.0489678	11.96
26	02-PressCapCube---ReC2---88	-665.0481517	12.47

27	02-PressCapCube---ReC2---80	-665.0439853	15.09
28	02-PressCapCube---ReC2---79	-665.0351045	20.66
29	02-PressCapCube---ReC2---89	-665.0288120	24.61
30	02-PressCapCube---ReC2---96	-665.0288120	24.61
31	03-Tl99---ReC2---172	-665.0286116	24.73
32	04-TrTrPr---ReC2---237	-665.0227972	28.38
33	04-TrTrPr---ReC2---240	-665.0227972	28.38
34	02-PressCapCube---ReC2---101	-665.0224139	28.62
35	01-CapCube---ReC2---6	-665.0213111	29.31
36	03-Tl99---ReC2---188	-665.0212431	29.36
37	04-TrTrPr---ReC2---243	-665.0212367	29.36
38	03-Tl99---ReC2---173	-665.0204075	29.88
39	03-Tl99---ReC2---203	-665.0204075	29.88
40	03-Tl99---ReC2---128	-665.0204004	29.89
41	03-Tl99---ReC2---134	-665.0204004	29.89
42	01-CapCube---ReC2---5	-665.0194386	30.49
43	04-TrTrPr---ReC2---258	-665.0194370	30.49
44	04-TrTrPr---ReC2---255	-665.0194005	30.51
45	02-PressCapCube---ReC2---120	-665.0183088	31.20
46	02-PressCapCube---ReC2---113	-665.0183078	31.20
47	04-TrTrPr---ReC2---270	-665.0183049	31.20
48	04-TrTrPr---ReC2---277	-665.0183049	31.20
49	03-Tl99---ReC2---226	-665.0183040	31.20
50	02-PressCapCube---ReC2---51	-665.0182956	31.21
51	03-Tl99---ReC2---133	-665.0182639	31.23
52	02-PressCapCube---ReC2---87	-665.0161007	32.58
53	02-PressCapCube---ReC2---102	-665.0156019	32.90
54	02-PressCapCube---ReC2---93	-665.0156009	32.90

55	03-Tl99---ReC2---155	-665.0155346	32.94
56	03-Tl99---ReC2---175	-665.0143568	33.68
57	02-PressCapCube---ReC2---58	-665.0137806	34.04
58	03-Tl99---ReC2---197	-665.0137763	34.04
59	02-PressCapCube---ReC2---77	-665.0137741	34.04
60	01-CapCube---ReC2---17	-665.0136041	34.15
61	01-CapCube---ReC2---28	-665.0136041	34.15
62	02-PressCapCube---ReC2---94	-665.0135811	34.17
63	02-PressCapCube---ReC2---112	-665.0125850	34.79
64	03-Tl99---ReC2---208	-665.0125635	34.80
65	03-Tl99---ReC2---230	-665.0125635	34.80
66	03-Tl99---ReC2---130	-665.0125449	34.82
67	04-TrTrPr---ReC2---269	-665.0120485	35.13
68	01-CapCube---ReC2---4	-665.0114380	35.51
69	01-CapCube---ReC2---8	-665.0114380	35.51
70	02-PressCapCube---ReC2---92	-665.0113383	35.57
71	01-CapCube---ReC2---41	-665.0103923	36.17
72	03-Tl99---ReC2---129	-665.0103843	36.17
73	02-PressCapCube---ReC2---71	-665.0103841	36.17
74	04-TrTrPr---ReC2---266	-665.0103784	36.18
75	04-TrTrPr---ReC2---294	-665.0103784	36.18
76	02-PressCapCube---ReC2---116	-665.0093855	36.80
77	04-TrTrPr---ReC2---276	-665.0087019	37.23
78	03-Tl99---ReC2---213	-665.0086966	37.23
79	03-Tl99---ReC2---222	-665.0086966	37.23
80	01-CapCube---ReC2---34	-665.0086656	37.25
81	01-CapCube---ReC2---13	-665.0086559	37.26
82	04-TrTrPr---ReC2---285	-665.0067331	38.46

83	01-CapCube---ReC2---36	-665.0066877	38.49
84	04-TrTrPr---ReC2---293	-665.0063827	38.68
85	02-PressCapCube---ReC2---109	-665.0063734	38.69
86	02-PressCapCube---ReC2---85	-665.0063728	38.69
87	03-Tl99---ReC2---217	-665.0063643	38.69
88	03-Tl99---ReC2---178	-665.0054212	39.29
89	01-CapCube---ReC2---22	-665.0054129	39.29
90	03-Tl99---ReC2---167	-665.0054107	39.29
91	03-Tl99---ReC2---148	-665.0053861	39.31
92	03-Tl99---ReC2---165	-665.0053861	39.31
93	03-Tl99---ReC2---171	-665.0040887	40.12
94	03-Tl99---ReC2---182	-665.0040887	40.12
95	03-Tl99---ReC2---169	-665.0037024	40.36
96	02-PressCapCube---ReC2---63	-665.0036760	40.38
97	01-CapCube---ReC2---42	-665.0036329	40.41
98	01-CapCube---ReC2---19	-665.0036292	40.41
99	04-TrTrPr---ReC2---281	-665.0007811	42.20
100	01-CapCube---ReC2---3	-664.9986214	43.55
101	04-TrTrPr---ReC2---239	-664.9985804	43.58
102	04-TrTrPr---ReC2---251	-664.9985804	43.58
103	04-TrTrPr---ReC2---242	-664.9985242	43.61
104	02-PressCapCube---ReC2---100	-664.9983748	43.71
105	02-PressCapCube---ReC2---52	-664.9973726	44.34
106	02-PressCapCube---ReC2---62	-664.9973726	44.34
107	02-PressCapCube---ReC2---90	-664.9973554	44.35
108	03-Tl99---ReC2---205	-664.9973399	44.36
109	03-Tl99---ReC2---179	-664.9969568	44.60
110	03-Tl99---ReC2---199	-664.9969568	44.60

111	02-PressCapCube---ReC2---110	-664.9969397	44.61
112	02-PressCapCube---ReC2---97	-664.9969366	44.61
113	03-Tl99---ReC2---207	-664.9969258	44.62
114	03-Tl99---ReC2---127	-664.9969256	44.62
115	03-Tl99---ReC2---141	-664.9969108	44.63
116	03-Tl99---ReC2---166	-664.9969108	44.63
117	01-CapCube---ReC2---27	-664.9968684	44.65
118	02-PressCapCube---ReC2---108	-664.9968431	44.67
119	04-TrTrPr---ReC2---260	-664.9968287	44.68
120	02-PressCapCube---ReC2---114	-664.9968187	44.68
121	02-PressCapCube---ReC2---57	-664.9967110	44.75
122	01-CapCube---ReC2---2	-664.9966109	44.81
123	03-Tl99---ReC2---153	-664.9965817	44.83
124	02-PressCapCube---ReC2---118	-664.9965569	44.85
125	04-TrTrPr---ReC2---265	-664.9964919	44.89
126	04-TrTrPr---ReC2---256	-664.9956995	45.39
127	04-TrTrPr---ReC2---252	-664.9948409	45.93
128	04-TrTrPr---ReC2---253	-664.9948409	45.93
129	01-CapCube---ReC2---12	-664.9948405	45.93
130	03-Tl99---ReC2---161	-664.9944987	46.14
131	03-Tl99---ReC2---206	-664.9942589	46.29
132	03-Tl99---ReC2---223	-664.9942589	46.29
133	02-PressCapCube---ReC2---50	-664.9940077	46.45
134	02-PressCapCube---ReC2---68	-664.9938108	46.57
135	03-Tl99---ReC2---136	-664.9932149	46.95
136	04-TrTrPr---ReC2---241	-664.9931530	46.98
137	02-PressCapCube---ReC2---76	-664.9931252	47.00
138	02-PressCapCube---ReC2---53	-664.9931202	47.01

139	02-PressCapCube---ReC2---56	-664.9925949	47.33
140	04-TrTrPr---ReC2---238	-664.9922798	47.53
141	04-TrTrPr---ReC2---254	-664.9922798	47.53
142	03-Tl99---ReC2---170	-664.9911796	48.22
143	03-Tl99---ReC2---189	-664.9911796	48.22
144	04-TrTrPr---ReC2---257	-664.9911469	48.24
145	04-TrTrPr---ReC2---244	-664.9911244	48.26
146	03-Tl99---ReC2---231	-664.9884655	49.93
147	03-Tl99---ReC2---187	-664.9877582	50.37
148	03-Tl99---ReC2---191	-664.9877582	50.37
149	03-Tl99---ReC2---211	-664.9872022	50.72
150	03-Tl99---ReC2---212	-664.9871986	50.72
151	02-PressCapCube---ReC2---119	-664.9868223	50.96
152	04-TrTrPr---ReC2---272	-664.9868089	50.97
153	04-TrTrPr---ReC2---292	-664.9868089	50.97
154	04-TrTrPr---ReC2---250	-664.9861440	51.38
155	04-TrTrPr---ReC2---249	-664.9861039	51.41
156	04-TrTrPr---ReC2---234	-664.9853883	51.86
157	03-Tl99---ReC2---131	-664.9840638	52.69
158	03-Tl99---ReC2---221	-664.9840282	52.71
159	03-Tl99---ReC2---227	-664.9840282	52.71
160	03-Tl99---ReC2---183	-664.9840096	52.72
161	03-Tl99---ReC2---138	-664.9839875	52.74
162	03-Tl99---ReC2---202	-664.9825746	53.62
163	03-Tl99---ReC2---220	-664.9825415	53.64
164	04-TrTrPr---ReC2---282	-664.9821329	53.90
165	01-CapCube---ReC2---32	-664.9821235	53.91
166	01-CapCube---ReC2---37	-664.9821235	53.91

167	03-Tl99---ReC2---156	-664.9818083	54.10
168	04-TrTrPr---ReC2---236	-664.9800771	55.19
169	04-TrTrPr---ReC2---261	-664.9790318	55.85
170	04-TrTrPr---ReC2---287	-664.9790318	55.85
171	03-Tl99---ReC2---150	-664.9790149	55.86
172	01-CapCube---ReC2---39	-664.9790057	55.86
173	04-TrTrPr---ReC2---262	-664.9787158	56.04
174	03-Tl99---ReC2---149	-664.9751860	58.26
175	04-TrTrPr---ReC2---286	-664.9749646	58.40
176	04-TrTrPr---ReC2---289	-664.9749646	58.40
177	02-PressCapCube---ReC2---70	-664.9749415	58.41
178	01-CapCube---ReC2---38	-664.9749284	58.42
179	01-CapCube---ReC2---25	-664.9749282	58.42
180	03-Tl99---ReC2---132	-664.9749222	58.42
181	04-TrTrPr---ReC2---278	-664.9748968	58.44
182	02-PressCapCube---ReC2---123	-664.9748942	58.44
183	01-CapCube---ReC2---35	-664.9744678	58.71
184	01-CapCube---ReC2---16	-664.9744667	58.71
185	03-Tl99---ReC2---162	-664.9737164	59.18
186	03-Tl99---ReC2---163	-664.9737033	59.19
187	01-CapCube---ReC2---43	-664.9731632	59.53
188	03-Tl99---ReC2---137	-664.9731249	59.55
189	01-CapCube---ReC2---9	-664.9716929	60.45
190	03-Tl99---ReC2---194	-664.9712155	60.75
191	03-Tl99---ReC2---201	-664.9712155	60.75
192	01-CapCube---ReC2---31	-664.9704469	61.23
193	03-Tl99---ReC2---219	-664.9701306	61.43
194	03-Tl99---ReC2---180	-664.9693740	61.91

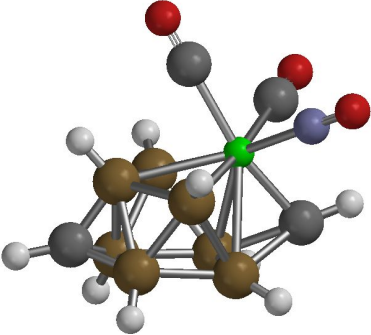
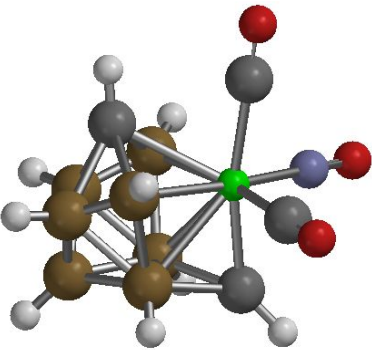
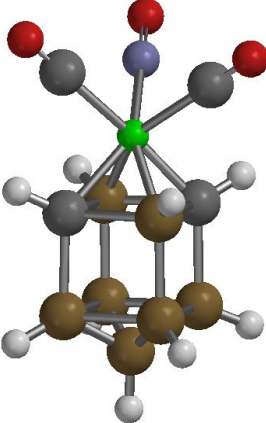
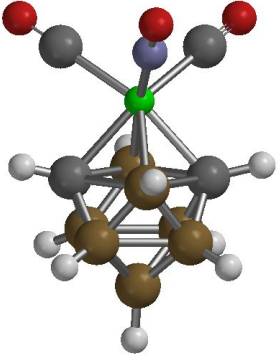
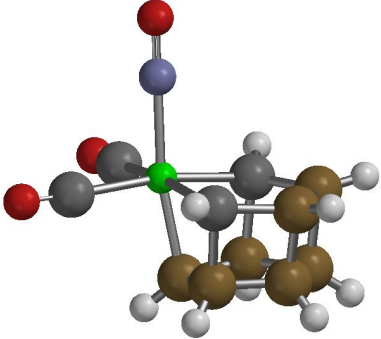
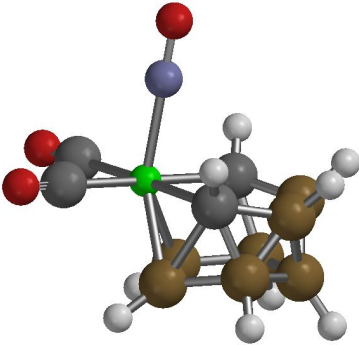
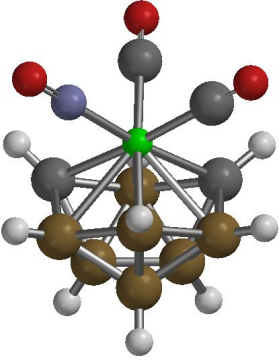
195	03-Tl99---ReC2---192	-664.9693740	61.91
196	03-Tl99---ReC2---135	-664.9692199	62.00
197	03-Tl99---ReC2---186	-664.9692040	62.01
198	03-Tl99---ReC2---198	-664.9692040	62.01
199	03-Tl99---ReC2---164	-664.9688035	62.26
200	03-Tl99---ReC2---200	-664.9687900	62.27
201	03-Tl99---ReC2---214	-664.9687699	62.29
202	04-TrTrPr---ReC2---248	-664.9687518	62.30
203	03-Tl99---ReC2---215	-664.9687211	62.32
204	03-Tl99---ReC2---229	-664.9687211	62.32
205	02-PressCapCube---ReC2---126	-664.9687173	62.32
206	01-CapCube---ReC2---26	-664.9682792	62.59
207	01-CapCube---ReC2---45	-664.9682774	62.59
208	03-Tl99---ReC2---218	-664.9678954	62.83
209	02-PressCapCube---ReC2---111	-664.9678697	62.85
210	02-PressCapCube---ReC2---54	-664.9664330	63.75
211	03-Tl99---ReC2---228	-664.9657118	64.20
212	04-TrTrPr---ReC2---288	-664.9648422	64.75
213	02-PressCapCube---ReC2---78	-664.9643901	65.03
214	01-CapCube---ReC2---48	-664.9643566	65.05
215	03-Tl99---ReC2---190	-664.9638411	65.38
216	04-TrTrPr---ReC2---267	-664.9636503	65.50
217	03-Tl99---ReC2---204	-664.9635943	65.53
218	01-CapCube---ReC2---47	-664.9635749	65.55
219	01-CapCube---ReC2---40	-664.9635739	65.55
220	03-Tl99---ReC2---154	-664.9632473	65.75
221	03-Tl99---ReC2---160	-664.9631942	65.78
222	04-TrTrPr---ReC2---268	-664.9625202	66.21

223	04-TrTrPr---ReC2---284	-664.9625202	66.21
224	04-TrTrPr---ReC2---279	-664.9616718	66.74
225	04-TrTrPr---ReC2---291	-664.9616718	66.74
226	03-Tl99---ReC2---142	-664.9610963	67.10
227	03-Tl99---ReC2---143	-664.9610604	67.12
228	01-CapCube---ReC2---1	-664.9608622	67.25
229	03-Tl99---ReC2---176	-664.9607650	67.31
230	03-Tl99---ReC2---210	-664.9607547	67.32
231	04-TrTrPr---ReC2---235	-664.9606411	67.39
232	02-PressCapCube---ReC2---64	-664.9603647	67.56
233	02-PressCapCube---ReC2---60	-664.9601507	67.69
234	03-Tl99---ReC2---140	-664.9598849	67.86
235	03-Tl99---ReC2---168	-664.9595997	68.04
236	03-Tl99---ReC2---139	-664.9595007	68.10
237	04-TrTrPr---ReC2---290	-664.9591224	68.34
238	02-PressCapCube---ReC2---121	-664.9586877	68.61
239	02-PressCapCube---ReC2---105	-664.9585236	68.72
240	04-TrTrPr---ReC2---274	-664.9568149	69.79
241	01-CapCube---ReC2---15	-664.9560105	70.29
242	03-Tl99---ReC2---209	-664.9552375	70.78
243	03-Tl99---ReC2---216	-664.9552375	70.78
244	02-PressCapCube---ReC2---106	-664.9551882	70.81
245	02-PressCapCube---ReC2---122	-664.9551882	70.81
246	04-TrTrPr---ReC2---264	-664.9551531	70.83
247	04-TrTrPr---ReC2---273	-664.9551531	70.83
248	02-PressCapCube---ReC2---74	-664.9538183	71.67
249	02-PressCapCube---ReC2---107	-664.9526285	72.41
250	02-PressCapCube---ReC2---115	-664.9526285	72.41

251	02-PressCapCube---ReC2---84	-664.9526127	72.42
252	03-Tl99---ReC2---225	-664.9514217	73.17
253	04-TrTrPr---ReC2---263	-664.9514145	73.18
254	04-TrTrPr---ReC2---280	-664.9514145	73.18
255	01-CapCube---ReC2---18	-664.9503735	73.83
256	01-CapCube---ReC2---29	-664.9493813	74.45
257	02-PressCapCube---ReC2---67	-664.9493143	74.49
258	02-PressCapCube---ReC2---75	-664.9493143	74.49
259	04-TrTrPr---ReC2---271	-664.9492063	74.56
260	03-Tl99---ReC2---185	-664.9482906	75.14
261	02-PressCapCube---ReC2---83	-664.9479302	75.36
262	02-PressCapCube---ReC2---91	-664.9479302	75.36
263	01-CapCube---ReC2---46	-664.9456517	76.79
264	04-TrTrPr---ReC2---275_i-33	-664.9450656	77.16
265	04-TrTrPr---ReC2---283_i-33	-664.9450656	77.16
266	04-TrTrPr---ReC2---275_r-33	-664.9449769	77.22
267	04-TrTrPr---ReC2---283_r-33	-664.9449769	77.22
268	03-Tl99---ReC2---177	-664.9445507	77.48
269	03-Tl99---ReC2---184	-664.9445507	77.48
270	01-CapCube---ReC2---33	-664.9431800	78.34
271	01-CapCube---ReC2---44	-664.9431800	78.34
272	03-Tl99---ReC2---193	-664.9427271	78.63
273	03-Tl99---ReC2---144	-664.9396421	80.56
274	03-Tl99---ReC2---159	-664.9396421	80.56
275	01-CapCube---ReC2---14	-664.9395974	80.59
276	03-Tl99---ReC2---147	-664.9395711	80.61
277	02-PressCapCube---ReC2---65_r-21	-664.9391580	80.87
278	02-PressCapCube---ReC2---99	-664.9390747	80.92

279	02-PressCapCube---ReC2---65_i-21	-664.9390658	80.93
280	02-PressCapCube---ReC2---125	-664.9370515	82.19
281	02-PressCapCube---ReC2---61	-664.9348241	83.59
282	02-PressCapCube---ReC2---66	-664.9348241	83.59
283	02-PressCapCube---ReC2---124	-664.9343333	83.90
284	02-PressCapCube---ReC2---69	-664.9340910	84.05
285	02-PressCapCube---ReC2---55	-664.9340829	84.05
286	03-Tl99---ReC2---146	-664.9336043	84.35
287	01-CapCube---ReC2---24	-664.9335980	84.36
288	03-Tl99---ReC2---145	-664.9335729	84.37
289	03-Tl99---ReC2---152	-664.9335729	84.37
290	01-CapCube---ReC2---23	-664.9300583	86.58
291	01-CapCube---ReC2---30	-664.9300583	86.58
292	02-PressCapCube---ReC2---72	-664.9294673	86.95
293	03-Tl99---ReC2---151	-664.9280019	87.87
294	03-Tl99---ReC2---158	-664.9280019	87.87
295	03-Tl99---ReC2---157	-664.9250228	89.74
296	02-PressCapCube---ReC2---59	-664.9117183	98.09
297	02-PressCapCube---ReC2---73	-664.9117183	98.09

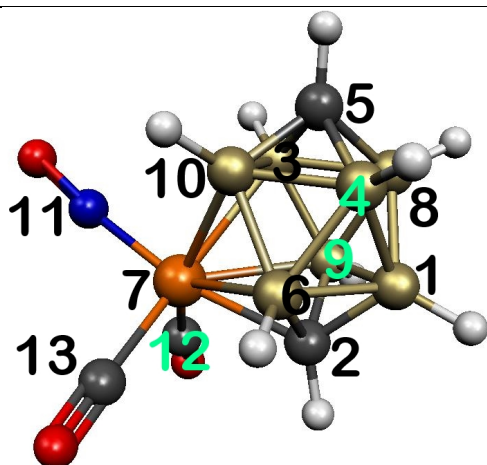
Table 3A. Initial $(\text{CO})_2(\text{NO})\text{ReC}_2\text{B}_7\text{H}_9$ structures (one example from each family), a total of 384 structures:

Initial structures	 1. Tetracapped trigonal prism (C_{2v}) 60 structures
 2. Tetracapped trigonal prism (C_{3v}) 36 structures	 3. Bicapped cube 80 structures
 4. Bicapped square antiprism 96 structures	 5. Pentagonal prism 8
	

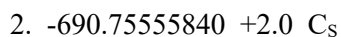
6. Pentagonal antiprism 8	7. Isocloso structure 96 structures
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Table 3B. Distances table for the lowest-lying (CO)₂(NO)ReC₂B₇H₉ structures after M06L/6-311G(d,p)//SDD optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry:

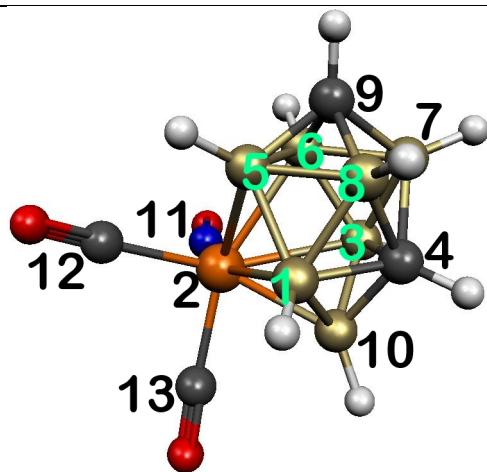
	1	2	3	4	5
1 B	0.000000				
2 C	1.580629	0.000000			
3 B	2.821373	2.855417	0.000000		
4 B	1.773228	2.771699	2.586321	0.000000	
5 C	2.734593	3.420458	1.590471	1.585752	0.000000
6 B	1.837128	1.618751	2.851894	1.810770	2.764301
7 Re	3.291099	2.154031	2.351429	3.538536	3.406904
8 B	1.774190	2.772037	1.807941	1.811518	1.585780
9 B	1.838265	1.619678	1.807321	2.820214	2.764977
10 B	2.822444	2.857276	1.888386	1.808568	1.589672
11 N	4.894585	3.970934	2.976851	4.659127	4.018784
12 C	4.364294	2.999961	3.569430	5.171416	4.976949
13 C	4.368315	3.012275	4.248897	4.637883	4.964454
	6	7	8	9	10
6 B	0.000000				
7 Re	2.370851	0.000000			
8 B	2.819813	3.538560	0.000000		
9 B	2.579838	2.371790	1.810861	0.000000	
10 B	1.808533	2.352951	2.586928	2.854358	0.000000
11 N	3.832053	1.841605	4.653436	3.823190	2.986351
12 C	4.009381	1.988667	4.648125	2.959914	4.255556
13 C	2.952435	1.988933	5.170409	4.019853	3.552547
	11	12	13		
11 N	0.000000				
12 C	2.846261	0.000000			
13 C	2.846516	2.860102	0.000000		



1. -690.75877310 0.0 C_s

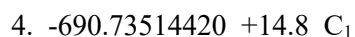


	1	2	3	4	5	
1 B	0.000000					
2 B	1.817468	0.000000				
3 C	2.761138	2.762701	0.000000			
4 B	1.811534	2.574131	2.845486	0.000000		
5 Re	3.545775	3.547147	2.132084	2.365639	0.000000	
6 B	2.574232	1.809699	2.846532	1.842166	2.368863	
7 B	1.769295	1.770508	1.581521	2.820409	3.290112	
8 B	2.819288	1.802702	1.614730	2.847719	2.384006	
9 B	1.804486	2.822005	1.612692	1.830903	2.380919	
10 C	1.585262	1.585636	3.421431	1.590942	3.446384	
11 N	5.071521	5.056584	2.829151	4.114496	1.843442	
12 C	4.392132	4.953473	3.782161	2.765543	1.987125	
13 C	4.937756	4.400643	3.814142	3.558154	1.989079	
	6	7	8	9	10	
6 B	0.000000					
7 B	2.820090	0.000000				
8 B	1.829090	1.832029	0.000000			
9 B	2.849962	1.833330	2.587719	0.000000		
10 C	1.591718	2.733658	2.778572	2.779827	0.000000	
11 N	4.096477	4.374535	3.512456	3.542371	5.228482	
12 C	3.602253	4.759819	4.242224	3.243808	4.241081	
13 C	2.754523	4.780126	3.285161	4.234251	4.213440	
	11	12	13			
11 N	0.000000					
12 C	2.814605	0.000000				
13 C	2.806479	2.824173	0.000000			

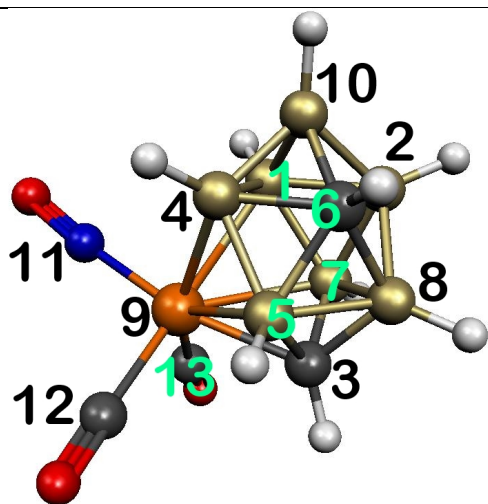


3. -690.74107820 +11.1 (Cs)

	1	2	3	4	5
1 B	0.000000				
2 Re	2.383522	0.000000			
3 B	2.594325	2.365801	0.000000		
4 C	1.721289	3.118289	1.725598	0.000000	
5 B	1.806586	2.349798	2.842950	2.669635	0.000000
6 B	2.859702	2.365307	1.811972	2.675154	1.872188
7 B	2.803810	3.506757	1.759802	1.690374	2.584260
8 B	1.767588	3.518054	2.803201	1.690091	1.808096
9 C	2.751074	3.422269	2.750436	2.603545	1.602637
10 B	1.744790	2.188115	1.734110	1.611781	3.000978
11 N	4.153352	1.837991	3.094625	4.475156	3.737756
12 C	3.327096	2.006456	4.234192	4.645086	2.747059
13 C	3.263981	1.990204	3.632652	4.101095	4.026783
	6	7	8	9	10
6 B	0.000000				
7 B	1.792450	0.000000			
8 B	2.580114	1.830552	0.000000		
9 C	1.590303	1.587129	1.580369	0.000000	
10 B	3.013044	2.892064	2.901597	3.581833	0.000000
11 N	2.933048	4.400683	4.980144	4.418014	3.569503
12 C	3.556546	4.924309	4.407032	4.201811	3.914390
13 C	4.273743	5.054431	4.878707	5.222429	2.590037
	11	12	13		
11 N	0.000000				
12 C	2.877581	0.000000			
13 C	2.880775	2.885229	0.000000		

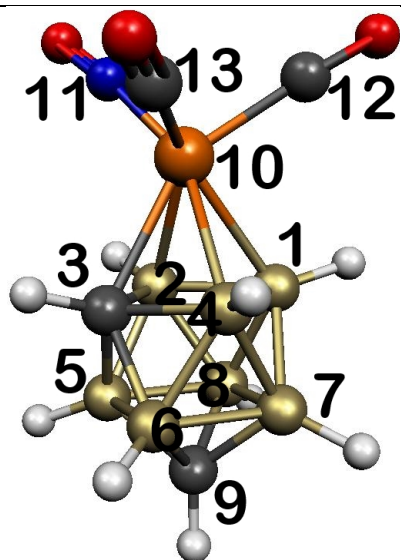


	1	2	3	4	5
1 C	0.000000				
2 B	2.712319	0.000000			
3 B	2.775285	1.819388	0.000000		
4 B	1.592708	2.775682	2.835387	0.000000	
5 Re	3.404838	3.276575	2.401485	2.310331	0.000000
6 C	2.641257	1.731324	2.481817	1.711318	2.339873
7 B	1.597504	1.759423	1.793613	2.576290	3.536002
8 B	3.557119	1.679218	1.726338	2.930967	2.189549
9 B	1.590854	2.796645	1.819584	1.872450	2.363428
10 B	1.579178	1.741421	2.810259	1.821358	3.538815
11 N	4.423290	4.613607	3.118682	3.723998	1.824163
12 C	4.170899	4.825913	4.270791	2.746293	2.006580
13 C	5.213110	4.234210	3.675262	3.980813	1.996249
	6	7	8	9	10
6 C	0.000000				
7 B	2.688816	0.000000			
8 B	1.661669	2.902006	0.000000		
9 B	2.735259	1.793545	2.981519	0.000000	
10 B	1.720531	1.804028	2.887874	2.578847	0.000000
11 N	4.077889	4.438601	3.550047	2.953067	4.998559
12 C	3.382810	4.944192	3.937297	3.549763	4.455863
13 C	3.282846	5.101601	2.625259	4.278922	4.906508
	11	12	13		
11 N	0.000000				
12 C	2.844103	0.000000			
13 C	2.851285	2.893969	0.000000		



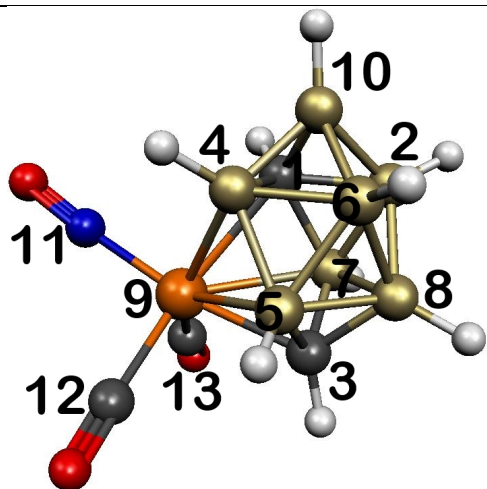
5. -690.73102860 +17.4 C₁

	1	2	3	4	5
1 B	0.000000				
2 B	1.803692	0.000000			
3 C	2.876098	2.756147	0.000000		
4 B	1.862860	2.565347	2.843394	0.000000	
5 B	2.849437	2.803752	1.609564	1.798020	0.000000
6 C	2.446100	1.716444	2.642121	1.711062	1.723571
7 B	1.828054	1.791398	1.621140	2.831941	2.567499
8 B	2.819999	1.747862	1.580099	2.804536	1.841207
9 Re	2.365886	3.525580	2.160435	2.334304	2.355011
10 B	1.685025	1.682254	3.579907	1.686705	2.899795
11 N	2.981983	4.641991	3.974094	2.957883	3.804058
12 C	4.265789	5.160384	3.011541	3.562724	2.955152
13 C	3.564609	4.622733	3.024695	4.229996	4.009702
	6	7	8	9	10
7 B	2.667684	0.000000			
8 B	1.684378	1.822557	0.000000		
9 Re	3.390082	2.377966	3.288193	0.000000	
10 B	1.620634	2.907145	2.856305	3.547019	0.000000
11 N	4.513494	3.834142	4.883732	1.839595	4.100267
12 C	4.536339	4.018161	4.373817	1.986452	5.114214
13 C	5.014886	2.959279	4.369504	1.992348	5.102677
	11	12	13		
11 N	0.000000				
12 C	2.840871	0.000000			
13 C	2.846186	2.869385	0.000000		



6. -690.72717660 +19.8 (Cs)

	1	2	3	4	5
1 B	0.000000				
2 B	1.812042	0.000000			
3 C	2.477390	1.717003	0.000000		
4 B	1.808578	2.506438	1.715087	0.000000	
5 B	2.820530	1.763263	1.685601	2.776886	0.000000
6 B	2.821493	2.774940	1.681101	1.767157	1.831181
7 B	1.793564	2.776399	2.665418	1.775038	2.577381
8 B	1.798062	1.774737	2.666443	2.777945	1.816501
9 C	2.759498	2.719881	2.599362	2.718444	1.590654
10 Re	2.278138	2.255311	2.291356	2.266147	3.594354
11 N	3.761742	3.027381	3.408778	4.007378	4.483712
12 C	2.914813	3.689822	4.115183	3.450296	5.212543
13 C	3.878133	4.019107	3.248390	2.971771	4.898732
	6	7	8	9	10
6 B	0.000000				
7 B	1.822757	0.000000			
8 B	2.577938	1.820296	0.000000		
9 C	1.588613	1.592310	1.593973	0.000000	
10 Re	3.599773	3.604685	3.600715	4.294722	0.000000
11 N	5.013866	5.219860	4.716733	5.585947	1.837080
12 C	5.093308	4.469361	4.607610	5.565343	1.965044
13 C	4.317727	4.710876	5.245565	5.501935	1.983414
	11	12	13		
11 N	0.000000				
12 C	2.806147	0.000000			
13 C	2.867304	2.839522	0.000000		



7. -690.72650270 +20.3 C₁

	1	2	3	4	5
1 C	0.000000				
2 B	1.702968	0.000000			
3 C	2.729363	2.761103	0.000000		
4 B	1.750850	2.548685	2.795700	0.000000	
5 B	2.728303	2.815429	1.612936	1.798406	0.000000
6 B	2.446767	1.809762	2.785308	1.804424	1.824051
7 B	1.700987	1.780159	1.609685	2.761400	2.559656
8 B	2.675697	1.760532	1.593305	2.778231	1.827402
9 Re	2.353613	3.564993	2.156983	2.304987	2.381451
10 B	1.618210	1.683571	3.577919	1.695295	2.925355
11 N	3.139974	4.742301	3.977060	2.962383	3.817459
12 C	4.243706	5.203114	2.988978	3.633261	3.035292
13 C	3.509778	4.607707	3.041566	4.163404	4.045497
	6	7	8	9	10
6 B	0.000000				
7 B	2.798343	0.000000			
8 B	1.778476	1.826644	0.000000		
9 Re	3.558019	2.399878	3.314878	0.000000	
10 B	1.682657	2.872804	2.871790	3.562462	0.000000
11 N	4.678090	3.907347	4.932857	1.842209	4.166313
12 C	4.732620	4.001769	4.394198	1.970620	5.190445
13 C	5.170589	2.955924	4.392709	1.988569	5.051100
	11	12	13		
11 N	0.000000				
12 C	2.787485	0.000000			
13 C	2.842043	2.825747	0.000000		

Table 3C. Energy ranking for (CO)₂(NO)ReC₂B₇H₉ obtained after B3LYP/6-31G(d)//SDD optimization:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	01-TetrcTriPri1----ReC2----66	-690.54353730	0.00
2	02-TetrcTriPri2----ReC2----227	-690.54352780	0.01
3	03-BicapCub----ReC2----366	-690.54351350	0.01
4	07-Isocloso----ReC2----524	-690.54351010	0.02
5	01-TetrcTriPri1----ReC2----51	-690.54350690	0.02
6	02-TetrcTriPri2----ReC2----186	-690.54350470	0.02
7	01-TetrcTriPri1----ReC2----36	-690.54350160	0.02
8	01-TetrcTriPri1----ReC2----11	-690.54349860	0.02
9	01-TetrcTriPri1----ReC2----79	-690.54049350	1.91
10	02-TetrcTriPri2----ReC2----278	-690.54047130	1.92
11	07-Isocloso----ReC2----499	-690.54045670	1.93
12	07-Isocloso----ReC2----494	-690.54045630	1.93
13	04-BicapSqAntipr----ReC2----432	-690.54044520	1.94
14	04-BicapSqAntipr----ReC2----472	-690.54044520	1.94
15	02-TetrcTriPri2----ReC2----266	-690.54043980	1.94
16	02-TetrcTriPri2----ReC2----198	-690.54043700	1.95
17	03-BicapCub----ReC2----328	-690.54043260	1.95
18	03-BicapCub----ReC2----352	-690.54043260	1.95
19	01-TetrcTriPri1----ReC2----57	-690.54041060	1.96
20	02-TetrcTriPri2----ReC2----256	-690.53839320	3.23
21	02-TetrcTriPri2----ReC2----291	-690.53839320	3.23
22	03-BicapCub----ReC2----329	-690.53832320	3.27
23	04-BicapSqAntipr----ReC2----467	-690.52046070	14.48
24	04-BicapSqAntipr----ReC2----447	-690.52046060	14.48
25	02-TetrcTriPri2----ReC2----273	-690.52042530	14.50
26	07-Isocloso----ReC2----565	-690.52041160	14.51

27	01-TetrcTriPri1----ReC2----149	-690.51946200	15.11
28	07-Isocloso----ReC2----498	-690.51945350	15.11
29	02-TetrcTriPri2----ReC2----196	-690.51945020	15.12
30	07-Isocloso----ReC2----534	-690.51944900	15.12
31	02-TetrcTriPri2----ReC2----264	-690.51944070	15.12
32	02-TetrcTriPri2----ReC2----294	-690.51944070	15.12
33	07-Isocloso----ReC2----517	-690.51943070	15.13
34	02-TetrcTriPri2----ReC2----232	-690.51942230	15.13
35	02-TetrcTriPri2----ReC2----180	-690.51938080	15.16
36	02-TetrcTriPri2----ReC2----168	-690.51937910	15.16
37	01-TetrcTriPri1----ReC2----111	-690.51937400	15.16
38	07-Isocloso----ReC2----521	-690.51771420	16.20
39	02-TetrcTriPri2----ReC2----202	-690.51766020	16.24
40	02-TetrcTriPri2----ReC2----276	-690.51729880	16.47
41	02-TetrcTriPri2----ReC2----229	-690.51729680	16.47
42	03-BicapCub----ReC2----308	-690.51729280	16.47
43	01-TetrcTriPri1----ReC2----122	-690.51729030	16.47
44	01-TetrcTriPri1----ReC2----153	-690.51729030	16.47
45	02-TetrcTriPri2----ReC2----282	-690.51727730	16.48
46	01-TetrcTriPri1----ReC2----47	-690.51725040	16.50
47	01-TetrcTriPri1----ReC2----74	-690.51724200	16.50
48	01-TetrcTriPri1----ReC2----156	-690.51511580	17.84
49	01-TetrcTriPri1----ReC2----107	-690.51511550	17.84
50	07-Isocloso----ReC2----525	-690.51511380	17.84
51	02-TetrcTriPri2----ReC2----231	-690.51511200	17.84
52	02-TetrcTriPri2----ReC2----162	-690.51510900	17.84
53	02-TetrcTriPri2----ReC2----193	-690.51510630	17.84
54	02-TetrcTriPri2----ReC2----274	-690.51510540	17.84

55	02-TetrcTriPri2----ReC2----250	-690.51510310	17.84
56	02-TetrcTriPri2----ReC2----249	-690.51510010	17.84
57	07-Isocloso----ReC2----503	-690.51509570	17.85
58	05-PentagPrism----ReC2----479	-690.51507330	17.86
59	07-Isocloso----ReC2----527	-690.51507050	17.86
60	01-TetrcTriPri1----ReC2----23	-690.51445870	18.25
61	01-TetrcTriPri1----ReC2----46	-690.51445600	18.25
62	02-TetrcTriPri2----ReC2----295	-690.51444470	18.26
63	02-TetrcTriPri2----ReC2----161	-690.51441000	18.28
64	01-TetrcTriPri1----ReC2----135	-690.51440180	18.28
65	01-TetrcTriPri1----ReC2----150	-690.51440180	18.28
66	04-BicapSqAntipr----ReC2----439	-690.51439960	18.28
67	04-BicapSqAntipr----ReC2----466	-690.51439960	18.28
68	02-TetrcTriPri2----ReC2----272	-690.51439500	18.29
69	02-TetrcTriPri2----ReC2----296	-690.51439190	18.29
70	02-TetrcTriPri2----ReC2----239	-690.51438870	18.29
71	02-TetrcTriPri2----ReC2----195	-690.51431620	18.34
72	02-TetrcTriPri2----ReC2----243	-690.51223010	19.65
73	02-TetrcTriPri2----ReC2----189	-690.51222110	19.65
74	07-Isocloso----ReC2----516	-690.51221120	19.66
75	02-TetrcTriPri2----ReC2----192	-690.51220360	19.66
76	02-TetrcTriPri2----ReC2----184	-690.51220250	19.66
77	02-TetrcTriPri2----ReC2----218	-690.51218760	19.67
78	02-TetrcTriPri2----ReC2----262	-690.51023760	20.90
79	02-TetrcTriPri2----ReC2----263	-690.51020770	20.91
80	02-TetrcTriPri2----ReC2----270	-690.51019880	20.92
81	04-BicapSqAntipr----ReC2----430	-690.51016920	20.94
82	04-BicapSqAntipr----ReC2----456	-690.51016920	20.94

83	04-BicapSqAntipr----ReC2----431	-690.50931750	21.47
84	07-Isocloso----ReC2----553	-690.50930150	21.48
85	07-Isocloso----ReC2----584	-690.50930150	21.48
86	07-Isocloso----ReC2----578	-690.50924620	21.52
87	02-TetrTriPri2----ReC2----210	-690.50823440	22.15
88	02-TetrTriPri2----ReC2----235	-690.50821850	22.16
89	01-TetrTriPri1----ReC2----137	-690.50821710	22.16
90	01-TetrTriPri1----ReC2----121	-690.50821620	22.16
91	02-TetrTriPri2----ReC2----191	-690.50819340	22.18
92	01-TetrTriPri1----ReC2----71	-690.50498220	24.19
93	01-TetrTriPri1----ReC2----144	-690.50497610	24.20
94	01-TetrTriPri1----ReC2----90	-690.50497610	24.20
95	04-BicapSqAntipr----ReC2----429	-690.50496620	24.20
96	04-BicapSqAntipr----ReC2----464	-690.50496620	24.20
97	01-TetrTriPri1----ReC2----59	-690.50494380	24.22
98	07-Isocloso----ReC2----507	-690.50494340	24.22
99	03-BicapCub----ReC2----316	-690.50470060	24.37
100	04-BicapSqAntipr----ReC2----460	-690.50383440	24.91
101	07-Isocloso----ReC2----491	-690.50383370	24.91
102	02-TetrTriPri2----ReC2----286	-690.50382590	24.92
103	07-Isocloso----ReC2----554	-690.50378380	24.95
104	02-TetrTriPri2----ReC2----175	-690.50377790	24.95
105	07-Isocloso----ReC2----571	-690.50377750	24.95
106	02-TetrTriPri2----ReC2----190	-690.50377360	24.95
107	07-Isocloso----ReC2----508	-690.50375350	24.97
108	02-TetrTriPri2----ReC2----269	-690.50375260	24.97
109	04-BicapSqAntipr----ReC2----428	-690.50374440	24.97
110	03-BicapCub----ReC2----315	-690.50329570	25.25

111	02-TetrcTriPri2----ReC2----252	-690.50040250	27.07
112	02-TetrcTriPri2----ReC2----251	-690.50035920	27.10
113	02-TetrcTriPri2----ReC2----283	-690.50035920	27.10
114	04-BicapSqAntipr----ReC2----455	-690.49329600	31.53
115	04-BicapSqAntipr----ReC2----470	-690.49329520	31.53
116	02-TetrcTriPri2----ReC2----258	-690.49329340	31.53
117	02-TetrcTriPri2----ReC2----257	-690.49326720	31.55
118	02-TetrcTriPri2----ReC2----277	-690.49326720	31.55
119	02-TetrcTriPri2----ReC2----224	-690.49325300	31.55
120	01-TetrcTriPri1----ReC2----84	-690.49324920	31.56
121	01-TetrcTriPri1----ReC2----78	-690.49324900	31.56
122	02-TetrcTriPri2----ReC2----226	-690.49324690	31.56
123	02-TetrcTriPri2----ReC2----200	-690.49324610	31.56
124	07-Isocloso----ReC2----502	-690.49322090	31.57
125	07-Isocloso----ReC2----518	-690.49321980	31.58
126	07-Isocloso----ReC2----532	-690.49320870	31.58
127	04-BicapSqAntipr----ReC2----471	-690.49293280	31.76
128	02-TetrcTriPri2----ReC2----230	-690.49292610	31.76
129	02-TetrcTriPri2----ReC2----248	-690.49292130	31.76
130	07-Isocloso----ReC2----535	-690.49291720	31.77
131	02-TetrcTriPri2----ReC2----280	-690.49291670	31.77
132	02-TetrcTriPri2----ReC2----289	-690.49291670	31.77
133	07-Isocloso----ReC2----522	-690.49291650	31.77
134	01-TetrcTriPri1----ReC2----127	-690.49289870	31.78
135	01-TetrcTriPri1----ReC2----145	-690.49289850	31.78
136	01-TetrcTriPri1----ReC2----27	-690.49288990	31.78
137	02-TetrcTriPri2----ReC2----290	-690.49287770	31.79
138	07-Isocloso----ReC2----566	-690.49255600	31.99

139	07-Isocloso----ReC2----574	-690.49255600	31.99
140	02-TetrcTriPri2----ReC2----167	-690.49252420	32.01
141	02-TetrcTriPri2----ReC2----188	-690.49252420	32.01
142	02-TetrcTriPri2----ReC2----185	-690.49252000	32.01
143	02-TetrcTriPri2----ReC2----199	-690.49252000	32.01
144	02-TetrcTriPri2----ReC2----281	-690.49250750	32.02
145	02-TetrcTriPri2----ReC2----275	-690.49250620	32.02
146	07-Isocloso----ReC2----500	-690.49250010	32.03
147	04-BicapSqAntipr----ReC2----468	-690.49241520	32.08
148	01-TetrcTriPri1----ReC2----151	-690.49100870	32.96
149	01-TetrcTriPri1----ReC2----119	-690.49099490	32.97
150	02-TetrcTriPri2----ReC2----201	-690.49097260	32.99
151	02-TetrcTriPri2----ReC2----194	-690.49096910	32.99
152	02-TetrcTriPri2----ReC2----177_r-50	-690.49094570	33.00
153	07-Isocloso----ReC2----497	-690.49091510	33.02
154	02-TetrcTriPri2----ReC2----247	-690.49080570	33.09
155	02-TetrcTriPri2----ReC2----228	-690.49072720	33.14
156	02-TetrcTriPri2----ReC2----240	-690.49072720	33.14
157	01-TetrcTriPri1----ReC2----130	-690.49069920	33.16
158	01-TetrcTriPri1----ReC2----141	-690.49069920	33.16
159	07-Isocloso----ReC2----495	-690.49069900	33.16
160	07-Isocloso----ReC2----523	-690.49069670	33.16
161	02-TetrcTriPri2----ReC2----170	-690.49069350	33.16
162	07-Isocloso----ReC2----512	-690.49064750	33.19
163	07-Isocloso----ReC2----528	-690.49064440	33.19
164	01-TetrcTriPri1----ReC2----60	-690.49061540	33.21
165	01-TetrcTriPri1----ReC2----80	-690.49061540	33.21
166	02-TetrcTriPri2----ReC2----178	-690.49006640	33.55

167	07-Isocloso----ReC2----519	-690.49005030	33.56
168	07-Isocloso----ReC2----526	-690.49005030	33.56
169	07-Isocloso----ReC2----492	-690.48982860	33.70
170	02-TetrTriPri2----ReC2----166	-690.48981100	33.71
171	07-Isocloso----ReC2----504	-690.48979070	33.73
172	07-Isocloso----ReC2----511	-690.48979070	33.73
173	01-TetrTriPri1----ReC2----143	-690.48977710	33.74
174	01-TetrTriPri1----ReC2----146	-690.48977710	33.74
175	02-TetrTriPri2----ReC2----169	-690.48972770	33.77
176	02-TetrTriPri2----ReC2----197	-690.48972770	33.77
177	02-TetrTriPri2----ReC2----265	-690.48970490	33.78
178	02-TetrTriPri2----ReC2----279	-690.48970490	33.78
179	04-BicapSqAntipr----ReC2----463	-690.48969560	33.79
180	04-BicapSqAntipr----ReC2----469	-690.48969560	33.79
181	07-Isocloso----ReC2----559	-690.48963640	33.82
182	07-Isocloso----ReC2----568	-690.48963640	33.82
183	01-TetrTriPri1----ReC2----54	-690.48925550	34.06
184	01-TetrTriPri1----ReC2----86	-690.48925550	34.06
185	01-TetrTriPri1----ReC2----82	-690.48922890	34.08
186	02-TetrTriPri2----ReC2----164	-690.48769250	35.04
187	07-Isocloso----ReC2----496	-690.48769010	35.05
188	01-TetrTriPri1----ReC2----77	-690.48766180	35.06
189	01-TetrTriPri1----ReC2----52	-690.48766050	35.06
190	02-TetrTriPri2----ReC2----174	-690.48765170	35.07
191	02-TetrTriPri2----ReC2----292	-690.48717880	35.37
192	02-TetrTriPri2----ReC2----293	-690.48706080	35.44
193	02-TetrTriPri2----ReC2----288	-690.48702920	35.46
194	02-TetrTriPri2----ReC2----215	-690.48649560	35.79

195	02-TetrTriPri2----ReC2----177_i-50	-690.48648390	35.80
196	01-TetrTriPri1----ReC2----25	-690.48601110	36.10
197	01-TetrTriPri1----ReC2----8	-690.48601110	36.10
198	01-TetrTriPri1----ReC2----48	-690.48600850	36.10
199	01-TetrTriPri1----ReC2----65	-690.48600560	36.10
200	01-TetrTriPri1----ReC2----152	-690.48599630	36.11
201	01-TetrTriPri1----ReC2----96	-690.48599220	36.11
202	03-BicapCub----ReC2----355	-690.48595530	36.13
203	03-BicapCub----ReC2----363	-690.48595530	36.13
204	01-TetrTriPri1----ReC2----87	-690.48586480	36.19
205	01-TetrTriPri1----ReC2----63	-690.48583510	36.21
206	01-TetrTriPri1----ReC2----88	-690.48583510	36.21
207	01-TetrTriPri1----ReC2----2	-690.48582940	36.21
208	01-TetrTriPri1----ReC2----32	-690.48582650	36.21
209	01-TetrTriPri1----ReC2----160	-690.48582270	36.22
210	01-TetrTriPri1----ReC2----91	-690.48582270	36.22
211	06-AntiPr----ReC2----482	-690.48581850	36.22
212	07-Isocloso----ReC2----563	-690.48523800	36.58
213	07-Isocloso----ReC2----557	-690.48517260	36.63
214	04-BicapSqAntipr----ReC2----444	-690.48477590	36.87
215	04-BicapSqAntipr----ReC2----459	-690.48477550	36.87
216	02-TetrTriPri2----ReC2----261	-690.48468110	36.93
217	02-TetrTriPri2----ReC2----220	-690.48465260	36.95
218	07-Isocloso----ReC2----546	-690.48464170	36.96
219	02-TetrTriPri2----ReC2----285	-690.48462860	36.97
220	02-TetrTriPri2----ReC2----260	-690.48462360	36.97
221	07-Isocloso----ReC2----572	-690.48461060	36.98
222	07-Isocloso----ReC2----549	-690.48460950	36.98

223	01-TetrcTriPri1----ReC2----120	-690.48406970	37.32
224	01-TetrcTriPri1----ReC2----95	-690.48406970	37.32
225	01-TetrcTriPri1----ReC2----1	-690.48406750	37.32
226	01-TetrcTriPri1----ReC2----68	-690.48403510	37.34
227	01-TetrcTriPri1----ReC2----76	-690.48403340	37.34
228	02-TetrcTriPri2----ReC2----204	-690.48343600	37.71
229	04-BicapSqAntipr----ReC2----457	-690.48286770	38.07
230	07-Isocloso----ReC2----505	-690.48274920	38.15
231	07-Isocloso----ReC2----576	-690.48273600	38.15
232	02-TetrcTriPri2----ReC2----287	-690.48273580	38.15
233	02-TetrcTriPri2----ReC2----268	-690.48273190	38.16
234	03-BicapCub----ReC2----321	-690.48270070	38.18
235	02-TetrcTriPri2----ReC2----205	-690.48269240	38.18
236	02-TetrcTriPri2----ReC2----171	-690.48269210	38.18
237	01-TetrcTriPri1----ReC2----114	-690.48269180	38.18
238	01-TetrcTriPri1----ReC2----142	-690.48269180	38.18
239	01-TetrcTriPri1----ReC2----33	-690.48268780	38.18
240	02-TetrcTriPri2----ReC2----206	-690.48268470	38.19
241	07-Isocloso----ReC2----489	-690.48265110	38.21
242	05-PentagPrism----ReC2----474	-690.48261810	38.23
243	05-PentagPrism----ReC2----476	-690.48258740	38.25
244	02-TetrcTriPri2----ReC2----246	-690.48258140	38.25
245	07-Isocloso----ReC2----537	-690.48255290	38.27
246	07-Isocloso----ReC2----583	-690.48255290	38.27
247	01-TetrcTriPri1----ReC2----134	-690.48180090	38.74
248	01-TetrcTriPri1----ReC2----118	-690.48179670	38.74
249	04-BicapSqAntipr----ReC2----438	-690.48179180	38.75
250	01-TetrcTriPri1----ReC2----7	-690.48112020	39.17

251	01-TetrcTriPri1----ReC2----30	-690.48080110	39.37
252	07-Isocloso----ReC2----531	-690.48079790	39.37
253	02-TetrcTriPri2----ReC2----238	-690.48050820	39.55
254	02-TetrcTriPri2----ReC2----165	-690.48048010	39.57
255	02-TetrcTriPri2----ReC2----172	-690.48046770	39.58
256	07-Isocloso----ReC2----509	-690.48042840	39.60
257	06-AntiPr----ReC2----488_i-10	-690.48035070	39.65
258	02-TetrcTriPri2----ReC2----216	-690.48033550	39.66
259	02-TetrcTriPri2----ReC2----225	-690.48033510	39.66
260	02-TetrcTriPri2----ReC2----259	-690.48033130	39.66
261	02-TetrcTriPri2----ReC2----253	-690.48033040	39.66
262	02-TetrcTriPri2----ReC2----211	-690.48032460	39.67
263	02-TetrcTriPri2----ReC2----233	-690.48031950	39.67
264	06-AntiPr----ReC2----488_r-10	-690.48030780	39.68
265	04-BicapSqAntipr----ReC2----427	-690.48030020	39.68
266	04-BicapSqAntipr----ReC2----448	-690.48030020	39.68
267	01-TetrcTriPri1----ReC2----4	-690.48029570	39.69
268	01-TetrcTriPri1----ReC2----125	-690.48029250	39.69
269	01-TetrcTriPri1----ReC2----129	-690.48028480	39.69
270	02-TetrcTriPri2----ReC2----254	-690.48027360	39.70
271	02-TetrcTriPri2----ReC2----255	-690.48026930	39.70
272	02-TetrcTriPri2----ReC2----267	-690.48026930	39.70
273	04-BicapSqAntipr----ReC2----426	-690.48026490	39.70
274	04-BicapSqAntipr----ReC2----440	-690.48026490	39.70
275	01-TetrcTriPri1----ReC2----136	-690.48025830	39.71
276	01-TetrcTriPri1----ReC2----94	-690.48025830	39.71
277	01-TetrcTriPri1----ReC2----55	-690.48005940	39.83
278	01-TetrcTriPri1----ReC2----58	-690.48002480	39.86

279	01-TetrcTriPri1----ReC2----139	-690.47973490	40.04
280	01-TetrcTriPri1----ReC2----98	-690.47973490	40.04
281	02-TetrcTriPri2----ReC2----284	-690.47963140	40.10
282	04-BicapSqAntipr----ReC2----423	-690.47945420	40.21
283	04-BicapSqAntipr----ReC2----462	-690.47918870	40.38
284	01-TetrcTriPri1----ReC2----75	-690.47901410	40.49
285	04-BicapSqAntipr----ReC2----435	-690.47883200	40.60
286	02-TetrcTriPri2----ReC2----221	-690.47795870	41.15
287	02-TetrcTriPri2----ReC2----242	-690.47795870	41.15
288	03-BicapCub----ReC2----318	-690.47795420	41.15
289	03-BicapCub----ReC2----319	-690.47795360	41.16
290	07-Isocloso----ReC2----506	-690.47750310	41.44
291	07-Isocloso----ReC2----536	-690.47749350	41.44
292	01-TetrcTriPri1----ReC2----9	-690.47745920	41.47
293	07-Isocloso----ReC2----493	-690.47745660	41.47
294	07-Isocloso----ReC2----515	-690.47745390	41.47
295	02-TetrcTriPri2----ReC2----219	-690.47743990	41.48
296	02-TetrcTriPri2----ReC2----234	-690.47743990	41.48
297	01-TetrcTriPri1----ReC2----106	-690.47743160	41.48
298	01-TetrcTriPri1----ReC2----140	-690.47743160	41.48
299	02-TetrcTriPri2----ReC2----173	-690.47740850	41.50
300	02-TetrcTriPri2----ReC2----183	-690.47740810	41.50
301	03-BicapCub----ReC2----299	-690.47686330	41.84
302	01-TetrcTriPri1----ReC2----132	-690.47680030	41.88
303	07-Isocloso----ReC2----501	-690.47671400	41.93
304	04-BicapSqAntipr----ReC2----433	-690.47664050	41.98
305	04-BicapSqAntipr----ReC2----452	-690.47633450	42.17
306	01-TetrcTriPri1----ReC2----6	-690.47554130	42.67

307	01-TetrcTriPri1----ReC2----24	-690.47554060	42.67
308	05-PentagPrism----ReC2----477	-690.47550150	42.69
309	01-TetrcTriPri1----ReC2----67	-690.47550050	42.69
310	03-BicapCub----ReC2----297	-690.47547200	42.71
311	01-TetrcTriPri1----ReC2----40	-690.47545620	42.72
312	01-TetrcTriPri1----ReC2----3	-690.47545080	42.73
313	01-TetrcTriPri1----ReC2----64	-690.47543280	42.74
314	03-BicapCub----ReC2----307	-690.47519680	42.89
315	07-Isocloso----ReC2----542	-690.47510900	42.94
316	07-Isocloso----ReC2----575	-690.47510900	42.94
317	07-Isocloso----ReC2----538	-690.47510250	42.94
318	03-BicapCub----ReC2----301	-690.47500620	43.00
319	01-TetrcTriPri1----ReC2----101	-690.47374530	43.80
320	03-BicapCub----ReC2----310	-690.47125010	45.36
321	03-BicapCub----ReC2----343	-690.46905070	46.74
322	03-BicapCub----ReC2----346	-690.46905070	46.74
323	07-Isocloso----ReC2----541	-690.46882660	46.88
324	07-Isocloso----ReC2----543	-690.46880730	46.89
325	07-Isocloso----ReC2----567	-690.46880730	46.89
326	02-TetrcTriPri2----ReC2----236	-690.46759250	47.66
327	01-TetrcTriPri1----ReC2----89	-690.46573870	48.82
328	01-TetrcTriPri1----ReC2----128	-690.46573660	48.82
329	07-Isocloso----ReC2----545	-690.46547230	48.99
330	07-Isocloso----ReC2----579	-690.46547230	48.99
331	01-TetrcTriPri1----ReC2----81	-690.46543990	49.01
332	02-TetrcTriPri2----ReC2----181	-690.46543340	49.01
333	01-TetrcTriPri1----ReC2----53	-690.46538030	49.05
334	01-TetrcTriPri1----ReC2----69	-690.46538030	49.05

335	07-Isocloso----ReC2----562	-690.46537010	49.05
336	01-TetrTriPri1----ReC2----49	-690.46536050	49.06
337	04-BicapSqAntipr----ReC2----465	-690.46534350	49.07
338	03-BicapCub----ReC2----345	-690.46534240	49.07
339	07-Isocloso----ReC2----573	-690.46531780	49.08
340	04-BicapSqAntipr----ReC2----379_r-14	-690.46510120	49.22
341	04-BicapSqAntipr----ReC2----386_r-14	-690.46510120	49.22
342	03-BicapCub----ReC2----298	-690.46504910	49.25
343	01-TetrTriPri1----ReC2----73	-690.46469450	49.48
344	04-BicapSqAntipr----ReC2----379_i-14	-690.46464970	49.50
345	04-BicapSqAntipr----ReC2----386_i-14	-690.46464970	49.50
346	02-TetrTriPri2----ReC2----223	-690.46449460	49.60
347	04-BicapSqAntipr----ReC2----445	-690.46448900	49.60
348	04-BicapSqAntipr----ReC2----451	-690.46448900	49.60
349	04-BicapSqAntipr----ReC2----454	-690.46439450	49.66
350	02-TetrTriPri2----ReC2----179	-690.46437840	49.67
351	03-BicapCub----ReC2----347	-690.46354010	50.20
352	03-BicapCub----ReC2----367	-690.46354010	50.20
353	07-Isocloso----ReC2----533	-690.46330660	50.35
354	07-Isocloso----ReC2----514	-690.46330340	50.35
355	07-Isocloso----ReC2----513	-690.46288570	50.61
356	07-Isocloso----ReC2----529	-690.46286850	50.62
357	02-TetrTriPri2----ReC2----208	-690.46285200	50.63
358	07-Isocloso----ReC2----569	-690.46280210	50.66
359	07-Isocloso----ReC2----581	-690.46280210	50.66
360	07-Isocloso----ReC2----577	-690.46277070	50.68
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362	04-BicapSqAntipr----ReC2----461	-690.46216950	51.06

363	04-BicapSqAntipr----ReC2----453	-690.46216540	51.06
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365	01-TetrcTriPri1----ReC2----154	-690.46215590	51.07
366	03-BicapCub----ReC2----356	-690.46211990	51.09
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368	02-TetrcTriPri2----ReC2----187	-690.46199020	51.17
369	02-TetrcTriPri2----ReC2----207	-690.46199020	51.17
370	02-TetrcTriPri2----ReC2----182	-690.46059120	52.05
371	07-Isocloso----ReC2----490	-690.46057720	52.06
372	07-Isocloso----ReC2----510	-690.46057260	52.06
373	07-Isocloso----ReC2----530	-690.46057200	52.06
374	07-Isocloso----ReC2----520	-690.46056830	52.06
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383	07-Isocloso----ReC2----558	-690.45935250	52.83
384	02-TetrcTriPri2----ReC2----222	-690.45858110	53.31
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386	04-BicapSqAntipr----ReC2----450	-690.45848090	53.37
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388	01-TetrcTriPri1----ReC2----131	-690.45845170	53.39
389	05-PentagPrism----ReC2----478	-690.45843820	53.40
390	01-TetrcTriPri1----ReC2----116	-690.45841590	53.42

391	07-Isocloso----ReC2----540	-690.45841070	53.42
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395	02-TetrTriPri2----ReC2----214	-690.45776000	53.83
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403	03-BicapCub----ReC2----311	-690.45505200	55.53
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405	07-Isocloso----ReC2----556	-690.45504870	55.53
406	07-Isocloso----ReC2----547	-690.45499480	55.56
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414	07-Isocloso----ReC2----539	-690.45095900	58.09
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416	07-Isocloso----ReC2----570	-690.45079810	58.20
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448	03-BicapCub----ReC2----375	-690.43609430	67.42
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450	01-TetrTriPri1----ReC2----108	-690.43607820	67.43
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452	03-BicapCub----ReC2----330	-690.43583210	67.59
453	03-BicapCub----ReC2----340	-690.43575320	67.64
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456	03-BicapCub----ReC2----365	-690.43561650	67.72
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461	03-BicapCub----ReC2----360	-690.43412460	68.66
462	03-BicapCub----ReC2----342	-690.43403970	68.71
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465	01-TetrTriPri1----ReC2----13	-690.43007960	71.20
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467	03-BicapCub----ReC2----357	-690.42947280	71.58
468	06-AntiPr----ReC2----484	-690.42894730	71.91
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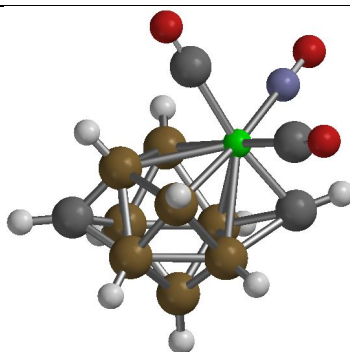
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521	03-BicapCub----ReC2----338	-690.41143380	82.90
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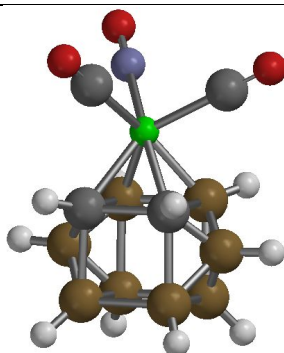
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575	01-TetrcTriPri1----ReC2----159	-690.37471770	105.94
576	01-TetrcTriPri1----ReC2----113	-690.36866860	109.73
577	01-TetrcTriPri1----ReC2----126	-690.36866860	109.73
578	01-TetrcTriPri1----ReC2----155	-690.36593450	111.45
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581	01-TetrcTriPri1----ReC2----26	-690.36225010	113.76
582	01-TetrcTriPri1----ReC2----123	-690.34748530	123.03
583	01-TetrcTriPri1----ReC2----97	-690.34748530	123.03
584	01-TetrcTriPri1----ReC2----110	-690.34305280	125.81
585	01-TetrcTriPri1----ReC2----117	-690.34301760	125.83
586	01-TetrcTriPri1----ReC2----115	-690.34128110	126.92

587	01-TetrcTriPri1----ReC2----158	-690.34128110	126.92
588	01-TetrcTriPri1----ReC2----18	-690.33749380	129.30
589	01-TetrcTriPri1----ReC2----29	-690.33749380	129.30
590	01-TetrcTriPri1----ReC2----16	-690.26994310	171.69
591	01-TetrcTriPri1----ReC2----5	-690.26994310	171.69

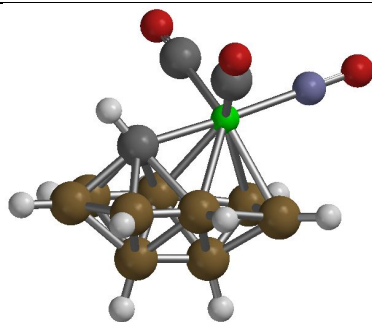
Table 4A. Initial $(\text{CO})_2(\text{NO})\text{ReC}_2\text{B}_8\text{H}_{10}$ structures (one example from each family), a total of 984 structures:



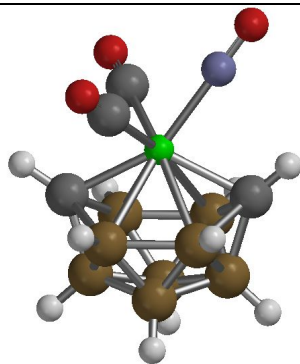
1. Pentacapped trigonal prism 88 structures



2. Tricapped cube 384 structures

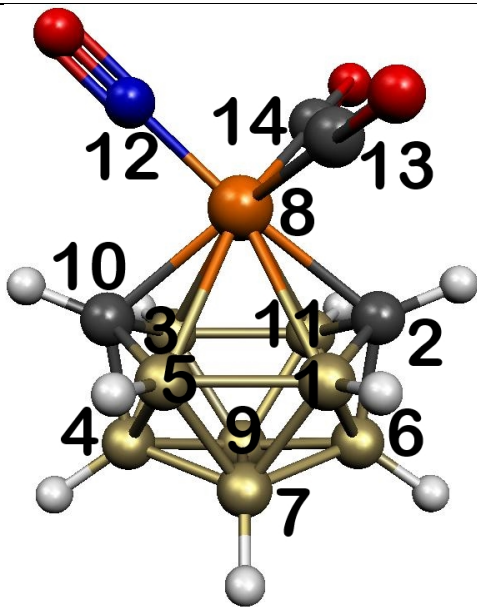


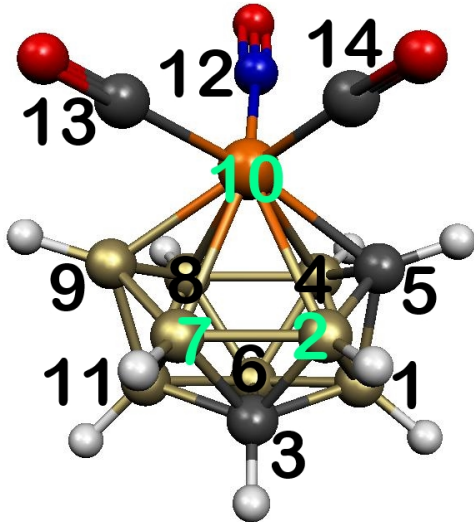
2b. Octahedron fused to pentag pyr 240 structures



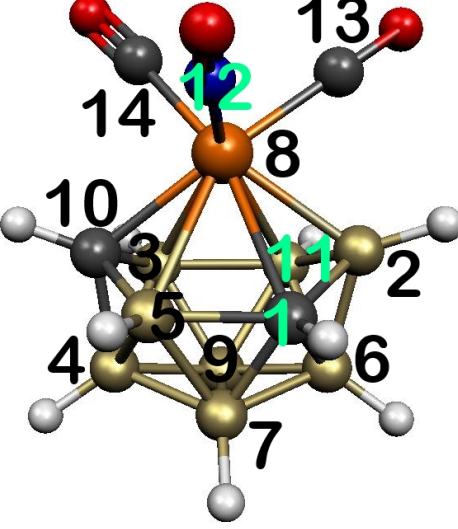
4. Edge-coalesced icosahedrons (icosahedron without a vertex) 272 structures

Table 4B. Distances table for the lowest-lying (CO)₂(NO)ReC₂B₈H₁₀ structures after M06L/6-311G(d,p)//SDD optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry:

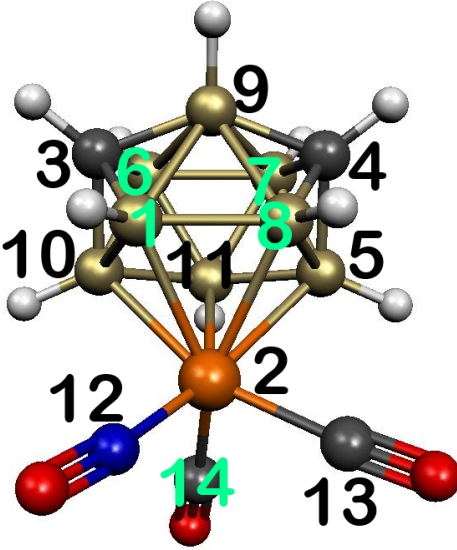
 1. -716.2067546 0.0 C_{2v}-C_s	1 2 3 4 5				
	1 B	0.000000			
	2 C	1.582223	0.000000		
	3 B	3.229983	2.970704	0.000000	
	4 B	2.950520	3.523009	1.815375	0.000000
	5 B	1.874859	2.968891	2.635478	1.816733
	6 B	1.809933	1.630489	2.962094	2.907828
	7 B	1.769298	2.711785	2.816857	1.739676
	8 Re	2.477798	2.205630	2.446898	3.309739
	9 B	2.808193	2.711907	1.775948	1.739968
	10 C	2.971847	3.368744	1.585585	1.619611
	11 B	2.620447	1.581802	1.872352	2.947417
	12 N	4.110567	4.047353	3.424478	4.269376
	13 C	2.818847	2.835125	4.378193	4.851357
	14 C	3.941935	2.836655	3.386296	4.842573
		6	7	8	9
	6 B	0.000000			
	7 B	1.742887	0.000000		
	8 Re	3.348255	3.428918	0.000000	
	9 B	1.743550	1.813098	3.428102	0.000000
	10 C	3.530064	2.709376	2.157148	2.708907
	11 B	1.810212	2.805481	2.473394	1.767487
	12 N	5.123240	4.868495	1.845486	4.867781
	13 C	4.233180	4.402928	2.004332	4.961486
	14 C	4.229658	4.957715	2.004022	4.391868
		11	12	13	14
	11 B	0.000000			
	12 N	4.106575	0.000000		

	13 C 3.936640 2.772088 0.000000					
	14 C 2.807878 2.772329 2.901427 0.000000					
 2. -716.1962432 +6.6 C₁	1 2 3 4 5					
	1 B	0.000000				
	2 B	1.804756	0.000000			
	3 C	1.661702	1.682317	0.000000		
	4 B	1.795349	2.623072	2.669712	0.000000	
	5 C	1.628811	1.593765	2.597044	1.584142	0.000000
	6 B	1.724758	2.789918	1.715184	1.761216	2.706430
	7 B	2.919601	1.817119	1.692473	3.214987	2.939150
	8 B	2.938379	3.214716	2.679848	1.871277	2.965331
	9 B	3.704359	3.123130	2.776650	3.136626	3.537008
	10 Re	3.302589	2.459128	3.266968	2.443215	2.175834
	11 B	2.884206	2.906118	1.671912	2.934142	3.498826
	12 N	4.506526	4.138683	4.817909	3.027522	3.271226
	13 C	5.043724	3.813602	4.463639	4.337589	4.084933
	14 C	4.223046	2.944767	4.432230	3.851638	2.746933
		6	7	8	9	10
	6 B	0.000000				
	7 B	2.802326	0.000000			
	8 B	1.766077	2.643827	0.000000		
	9 B	2.872329	1.732142	1.699084	0.000000	
	10 Re	3.384605	2.429707	2.415994	2.224071	0.000000
	11 B	1.742892	1.797430	1.796218	1.705771	3.247458
	12 N	4.368717	4.164493	3.057756	3.374703	1.837821
	13 C	4.869705	2.970695	3.603630	2.448335	2.007699
	14 C	4.978658	3.602032	4.398183	4.046726	2.041704
		11	12	13	14	
	11 B	0.000000				

	12 N 4.522930 0.000000				
	13 C 4.026495 2.825605 0.000000				
	14 C 4.951613 2.935678 2.788406 0.000000				
3. -716.1954398 +7.1 C_s	1 2 3 4 5				
	1 B 0.000000				
	2 C 1.582209 0.000000				
	3 B 3.218291 2.841047 0.000000				
	4 B 2.939079 3.446048 1.793459 0.000000				
	5 B 1.793775 2.766509 2.823263 1.759020 0.000000				
	6 B 1.986922 1.624494 1.974610 2.662378 2.778088				
	7 B 1.832579 2.842434 2.648976 1.792538 1.754280				
	8 Re 2.325094 2.212323 3.617190 3.600542 2.320995				
	9 C 2.831390 3.043160 1.562945 1.632893 2.679164				
	10 B 2.844568 2.766394 1.755334 1.757096 1.844185				
	11 B 2.643283 1.581564 1.831016 2.938572 2.845701				
	12 N 3.804375 4.023600 4.753110 4.314796 3.046448				
	13 C 2.827024 3.051765 5.315041 5.140291 3.532618				
	14 C 3.959401 3.067090 4.539205 5.134045 4.214290				
	6 7 8 9 10				
	6 B 0.000000				
	7 B 1.973614 0.000000				
	8 Re 3.398889 3.616180 0.000000				
	9 C 1.618270 1.562487 4.168203 0.000000				
	10 B 2.778852 2.821042 2.322276 2.678457 0.000000				
	11 B 1.988382 3.218315 2.327557 2.830975 1.795147				
	12 N 5.007247 4.741816 1.833513 5.386378 3.058056				
	13 C 4.456610 4.542457 1.994497 5.485360 4.217484				
	14 C 4.467806 5.319207 1.994797 5.487796 3.523143				
	11 12 13 14				

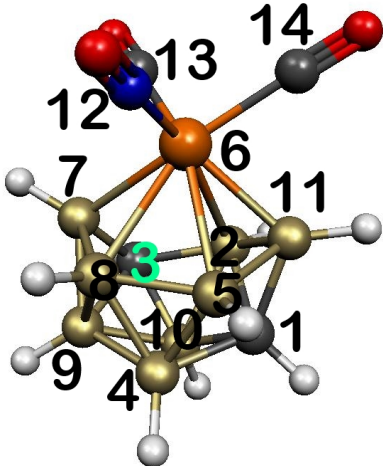
	11 B 0.000000 12 N 3.818611 0.000000 13 C 3.949718 2.827174 0.000000 14 C 2.830645 2.828423 2.889081 0.000000
 4. -716.1897511 +10.7 C₁	1 2 3 4 5 1 C 0.000000 2 B 1.601453 0.000000 3 B 3.081586 3.105445 0.000000 4 B 2.819108 3.665076 1.803461 0.000000 5 B 1.771360 3.040915 2.619722 1.807775 0.000000 6 B 1.731098 1.710250 2.905391 2.886996 2.920384 7 B 1.679794 2.821207 2.793430 1.739028 1.773141 8 Re 2.382041 2.224102 2.460926 3.300463 2.417630 9 B 2.689659 2.878365 1.766013 1.743128 2.808502 10 C 2.849371 3.486770 1.609137 1.630388 1.578196 11 B 2.527239 1.731229 1.839029 2.940202 3.202494 12 N 3.177453 3.417140 4.147493 4.531146 3.053641 13 C 3.555118 2.435070 3.796082 5.021754 4.289376 14 C 4.320073 4.010789 2.944263 4.228981 3.853759 6 7 8 9 10 6 B 0.000000 7 B 1.729316 0.000000 8 Re 3.289318 3.408307 0.000000 9 B 1.726470 1.799454 3.434986 0.000000 10 C 3.503760 2.717702 2.151965 2.734334 0.000000 11 B 1.793131 2.803609 2.455469 1.784449 2.960537 12 N 4.625808 4.455372 1.842682 5.029609 3.248538 13 C 4.011394 4.846506 2.011364 4.560706 4.065324 14 C 4.948587 4.990431 2.006961 4.548057 2.763837

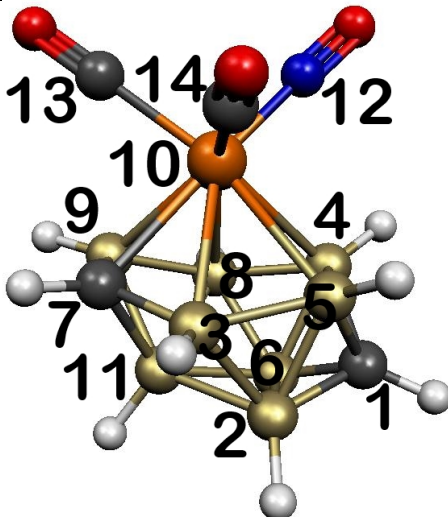
	11	12	13	14
	11 B	0.000000		
	12 N	4.210818	0.000000	
	13 C	2.933671	2.846834	0.000000
	14 C	3.590082	2.866025	2.760710

 5. -716.1887825 +11.3 (Cs)	1	2	3	4	5	
	1 B	0.000000				
	2 Re	2.300107	0.000000			
	3 C	1.560516	3.356095	0.000000		
	4 C	2.830757	3.356437	3.014419	0.000000	
	5 B	3.013232	2.328290	3.436200	1.642143	0.000000
	6 B	2.662045	3.540651	1.561474	2.810431	2.929636
	7 B	3.230997	3.549625	2.806388	1.559598	1.773530
	8 B	1.860596	2.315518	2.841248	1.560063	1.877916
	9 B	1.993925	3.535379	1.617145	1.619264	2.694848
	10 B	1.858810	2.325902	1.637832	3.437459	3.026218
	11 B	2.863446	2.403463	2.696922	2.692678	1.783645
	12 N	2.853532	1.840536	4.115857	4.876788	4.124536
	13 C	3.799936	1.990922	5.038671	3.892022	2.807804
	14 C	4.061118	1.988279	4.699662	4.790398	3.329190

	6	7	8	9	10
6 B	0.000000				
7 B	1.808655	0.000000			
8 B	3.243910	2.673121	0.000000		
9 B	1.971087	1.964521	1.998692	0.000000	
10 B	1.768871	2.939027	3.026980	2.692226	0.000000
11 B	1.764822	1.771004	2.877564	2.776573	1.798918
12 N	4.787912	5.206435	3.524099	4.692570	3.179382
13 C	5.152559	4.525854	2.860725	4.697947	4.259200

	14 C 4.392486 4.462861 4.141564 5.085162 3.200130 11 12 13 14 11 B 0.000000 12 N 4.017082 0.000000 13 C 3.823344 2.876728 0.000000 14 C 2.858359 2.850068 2.874432 0.000000
6. -716.1870837 +12.3 C₁	1 2 3 4 5 1 B 0.000000 2 C 2.710101 0.000000 3 B 2.783612 1.622172 0.000000 4 B 1.755518 2.837942 2.012284 0.000000 5 B 1.799712 2.756493 2.820593 2.821060 0.000000 6 Re 3.551637 2.143772 2.648453 4.021366 2.324828 7 B 2.815557 2.920798 2.067552 2.665802 1.791845 8 B 1.748594 3.434873 2.699059 1.767669 1.778152 9 C 2.673361 3.020027 1.622007 1.567031 2.695869 10 B 1.752218 1.568245 1.983522 1.810348 2.817942 11 B 1.778277 1.664932 2.683044 2.931106 1.801492 12 N 4.606945 3.918237 4.298721 5.368470 2.921664 13 C 5.095825 3.252850 3.120190 4.961037 3.956759 14 C 4.882992 2.850221 4.008566 5.495028 3.989493 6 7 8 9 10 6 Re 0.000000 7 B 2.365741 0.000000 8 B 3.625544 1.777433 0.000000 9 C 3.477046 1.558942 1.649554 0.000000 10 B 3.382781 3.249436 2.898843 2.791870 0.000000 11 B 2.349966 2.982392 2.954907 3.397129 1.780790 12 N 1.837938 3.188878 4.415377 4.670553 4.961635

	12 N	4.654523	4.333853	1.833423	5.134836	3.332122
	13 C	4.138190	4.829289	2.014167	4.885623	4.171302
	14 C	4.803257	4.744000	2.015207	4.532446	2.553733
		11	12	13	14	
	11 B	0.000000				
	12 N	4.280225	0.000000			
	13 C	3.260666	2.873810	0.000000		
	14 C	3.351675	2.925198	2.831055	0.000000	
 8. -716.1803568 +16.6 C₁ 3-6 fragile edge		1	2	3	4	5
	1 C	0.000000				
	2 B	1.796800	0.000000			
	3 C	2.697600	1.671125	0.000000		
	4 B	1.660712	2.785841	2.697398	0.000000	
	5 B	1.697311	2.670860	3.289304	1.750461	0.000000
	6 Re	3.150970	2.493593	3.006012	3.469795	2.373826
	7 B	3.333352	2.592600	1.591630	2.855601	3.064656
	8 B	2.730071	2.994372	2.617900	1.791106	1.815961
	9 B	2.759085	2.789645	1.669031	1.734947	2.930513
	10 B	1.678595	1.833602	1.609967	1.780025	2.845949
	11 B	1.618542	1.742022	3.149267	2.864469	1.755575
	12 N	4.552467	4.279948	4.516380	4.435335	3.195190
	13 C	4.630495	3.273426	3.258614	4.906146	4.256341
	14 C	4.107308	3.389440	4.510756	5.004896	3.587647
		6	7	8	9	10
	6 Re	0.000000				
	7 B	2.319008	0.000000			
	8 B	2.377483	1.734602	0.000000		
	9 B	3.492230	1.745143	1.793842	0.000000	
	10 B	3.686234	2.749779	2.793373	1.737535	0.000000

	11 B	2.152154	3.424240	3.020513	3.657432	2.898138
	12 N	1.837682	3.319419	2.927283	4.520814	5.168957
	13 C	2.009044	2.582645	3.692228	4.235253	4.574880
	14 C	2.011582	4.220161	4.280453	5.314402	5.023551
	11	12	13	14		
	11 B	0.000000				
	12 N	3.631556	0.000000			
9. -716.1784069 +17.8 C₁	13 C	3.752374	2.926069	0.000000		
	14 C	2.538206	2.874116	2.849025	0.000000	
	1	2	3	4	5	
	1 C	0.000000				
	2 B	1.574743	0.000000			
	3 B	2.800737	1.771137	0.000000		
	4 B	1.583635	2.562015	3.000078	0.000000	
	5 B	1.587452	1.793018	1.807435	1.877780	0.000000
	6 B	1.576893	1.795242	2.930409	1.780152	2.561598
	7 C	3.780862	2.847851	1.561928	3.446397	3.002192
	8 B	2.779004	2.912398	3.017932	1.778106	2.959924
	9 B	3.920129	3.415027	2.735270	3.131957	3.557187
	10 Re	3.455940	3.474829	2.444232	2.430355	2.410396
	11 B	2.823173	1.869386	1.954410	2.836815	2.840663
	12 N	4.103618	4.733222	4.091187	2.748125	3.319553
13 C	5.355637	5.154491	3.854777	4.211341	4.367647	
14 C	4.455691	4.283193	2.858877	3.912930	2.929053	
6	7	8	9	10		
6 B	0.000000					
7 C	3.285320	0.000000				
8 B	1.759805	2.635522	0.000000			
9 B	2.980631	1.527180	1.676826	0.000000		

	10 Re 3.475056 2.265844 2.425481 2.317969 0.000000
	11 B 1.862557 1.722238 1.941160 1.825813 3.056495
	12 N 4.355922 4.075634 3.288139 3.753997 1.833522
	13 C 5.014484 2.890775 3.524671 2.618572 2.003009
	14 C 4.966384 3.186098 4.321358 3.963127 1.998819
	11 12 13 14
	11 B 0.000000
	12 N 4.571110 0.000000
	13 C 4.148229 2.812585 0.000000
	14 C 4.376752 2.848459 2.890001 0.000000
	1 2 3 4 5
	1 Re 0.000000
10. -716.1760563 +19.3 (C _s)	2 B 2.474383 0.000000
	3 B 3.440594 2.833783 0.000000
	4 B 2.353693 2.657315 2.915240 0.000000
	5 B 3.260996 1.856505 2.874058 1.799910 0.000000
	6 B 3.451599 2.790808 1.718916 1.770957 1.740237
	7 B 3.599060 1.803279 1.727805 2.840135 1.751754
	8 B 2.149637 1.757812 3.689060 1.744383 1.707186
	9 C 2.367161 2.944808 1.706999 1.748736 2.764595
	10 B 2.265258 2.757006 1.732828 2.995374 3.510177
	11 C 2.799306 1.712716 1.670592 3.198715 2.821962
	12 N 1.836705 4.261215 4.587718 3.124660 4.623065
	13 C 1.992300 3.201469 5.202567 3.612596 4.128585
	14 C 2.025520 3.398025 4.188186 4.261548 4.823577
	6 7 8 9 10
	6 B 0.000000
	7 B 1.785345 0.000000
	8 B 2.893840 2.923531 0.000000

	9 C	1.693377	2.664124	2.971853	0.000000	
	10 B	2.816203	2.774977	3.484112	1.616990	0.000000
	11 C	2.678726	1.643094	3.130278	2.442316	1.589317
	12 N	4.462692	5.141684	3.501029	3.072552	3.334610
	13 C	4.975734	4.845944	2.483353	4.257544	4.131408
	14 C	4.904796	4.541996	3.862477	3.672255	2.572620
		11	12	13	14	
	11 C	0.000000				
	12 N	4.399476	0.000000			
	13 C	4.206425	2.833574	0.000000		
	14 C	3.113020	2.940334	2.805030	0.000000	

Table 4C. Energy ranking for (CO)₂(NO)ReC₂B₈H₁₀ obtained after B3LYP/6-31G(d)//SDD optimization.

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	04-Icos-1vx---ReC2-----776	-715.9864839	0.00
2	04-Icos-1vx---ReC2-----746	-715.9864807	0.00
3	02-TricapCubeB---ReC2-----296	-715.9864586	0.02
4	02-TricapCubeB---ReC2-----263	-715.9864572	0.02
5	02-TricapCubeB---ReC2-----360	-715.9864555	0.02
6	04-Icos-1vx---ReC2-----775	-715.9732712	8.29
7	04-Icos-1vx---ReC2-----810	-715.9732712	8.29
8	04-Icos-1vx---ReC2-----958	-715.9732455	8.31
9	04-Icos-1vx---ReC2-----970	-715.9732455	8.31
10	02-TricapCubeA---ReC2-----203	-715.9732144	8.33
11	02-TricapCubeB---ReC2-----343	-715.9705324	10.01
12	02-TricapCubeB---ReC2-----348	-715.9705324	10.01
13	02-TricapCubeB---ReC2-----344	-715.9705160	10.02
14	02-TricapCubeA---ReC2-----196	-715.9705025	10.03
15	04-Icos-1vx---ReC2-----767	-715.9704932	10.03
16	02-TricapCubeB---ReC2-----269	-715.9704924	10.03
17	04-Icos-1vx---ReC2-----809	-715.9704920	10.04
18	02-TricapCubeB---ReC2-----283	-715.9704917	10.04
19	04-Icos-1vx---ReC2-----929	-715.9704830	10.04
20	04-Icos-1vx---ReC2-----953	-715.9704823	10.04
21	02-TricapCubeB---ReC2-----400	-715.9704820	10.04
22	04-Icos-1vx---ReC2-----784	-715.9704764	10.05
23	02-TricapCubeB---ReC2-----287	-715.9704427	10.07
24	02-TricapCubeB---ReC2-----405	-715.9704358	10.07
25	02-TricapCubeB---ReC2-----398	-715.9704350	10.07

26	02-TricapCubeA----ReC2-----207	-715.9696960	10.53
27	02-TricapCubeA----ReC2-----250	-715.9696592	10.56
28	01-PentaCapTrPr----ReC2-----53	-715.9696547	10.56
29	01-PentaCapTrPr----ReC2-----13	-715.9696526	10.56
30	04-Icos-1vx----ReC2-----880	-715.9696478	10.56
31	04-Icos-1vx----ReC2-----770	-715.9695698	10.61
32	04-Icos-1vx----ReC2-----786	-715.9695698	10.61
33	01-PentaCapTrPr----ReC2-----19	-715.9695061	10.65
34	02-TricapCubeB----ReC2-----315	-715.9693901	10.73
35	02-TricapCubeB----ReC2-----337	-715.9693892	10.73
36	02-TricapCubeB----ReC2-----393	-715.9693285	10.77
37	02-TricapCubeA----ReC2-----188	-715.9693251	10.77
38	02-TricapCubeB----ReC2-----372	-715.9693237	10.77
39	02-TricapCubeB----ReC2-----282	-715.9692953	10.79
40	03-OhfusetopentBipyr----ReC2-----556	-715.9683555	11.38
41	03-OhfusetopentBipyr----ReC2-----531	-715.9683536	11.38
42	04-Icos-1vx----ReC2-----752	-715.9683035	11.41
43	04-Icos-1vx----ReC2-----816	-715.9683035	11.41
44	02-TricapCubeA----ReC2-----94	-715.9682864	11.42
45	04-Icos-1vx----ReC2-----942	-715.9682417	11.45
46	04-Icos-1vx----ReC2-----878	-715.9682139	11.46
47	02-TricapCubeB----ReC2-----410	-715.9682052	11.47
48	02-TricapCubeB----ReC2-----354	-715.9681961	11.48
49	02-TricapCubeB----ReC2-----333	-715.9679190	11.65
50	04-Icos-1vx----ReC2-----751	-715.9678659	11.68
51	04-Icos-1vx----ReC2-----808	-715.9678651	11.68
52	02-TricapCubeA----ReC2-----134	-715.9677020	11.79
53	02-TricapCubeB----ReC2-----276	-715.9676989	11.79

54	03-OhfusetopentBipyr----ReC2-----562	-715.9676945	11.79
55	04-Icos-1vx----ReC2-----939	-715.9676537	11.82
56	02-TricapCubeB----ReC2-----407	-715.9676518	11.82
57	02-TricapCubeB----ReC2-----391	-715.9676515	11.82
58	01-PentaCapTrPr----ReC2-----83	-715.9676428	11.82
59	02-TricapCubeB----ReC2-----392	-715.9676299	11.83
60	02-TricapCubeB----ReC2-----261	-715.9676074	11.85
61	01-PentaCapTrPr----ReC2-----31	-715.9676068	11.85
62	02-TricapCubeB----ReC2-----323_r-28	-715.9676058	11.85
63	02-TricapCubeB----ReC2-----365_r-29	-715.9676052	11.85
64	01-PentaCapTrPr----ReC2-----7	-715.9676044	11.85
65	02-TricapCubeB----ReC2-----351	-715.9676042	11.85
66	02-TricapCubeA----ReC2-----199	-715.9676029	11.85
67	02-TricapCubeB----ReC2-----335	-715.9675983	11.85
68	04-Icos-1vx----ReC2-----943	-715.9675863	11.86
69	02-TricapCubeB----ReC2-----336	-715.9675688	11.87
70	02-TricapCubeA----ReC2-----118	-715.9674153	11.97
71	01-PentaCapTrPr----ReC2-----43	-715.9673468	12.01
72	02-TricapCubeA----ReC2-----241_i-29	-715.9669730	12.24
73	02-TricapCubeA----ReC2-----214_i-28	-715.9669720	12.24
74	03-OhfusetopentBipyr----ReC2-----561_i-13	-715.9669630	12.25
75	02-TricapCubeB----ReC2-----378_r-25	-715.9669496	12.26
76	02-TricapCubeB----ReC2-----418	-715.9669298	12.27
77	03-OhfusetopentBipyr----ReC2-----561_r-13	-715.9669232	12.27
78	02-TricapCubeB----ReC2-----322	-715.9669048	12.29
79	03-OhfusetopentBipyr----ReC2-----485	-715.9669014	12.29
80	04-Icos-1vx----ReC2-----736	-715.9669002	12.29

81	03-OhfusetopentBipyr----ReC2-----564	-715.9668938	12.29
82	01-PentaCapTrPr----ReC2-----52	-715.9668895	12.30
83	03-OhfusetopentBipyr----ReC2-----525	-715.9668893	12.30
84	02-TricapCubeA----ReC2-----214_r-28	-715.9668823	12.30
85	02-TricapCubeA----ReC2-----241_r-29	-715.9668822	12.30
86	02-TricapCubeB----ReC2-----421	-715.9668805	12.30
87	04-Icos-1vx----ReC2-----797	-715.9668802	12.30
88	04-Icos-1vx----ReC2-----820	-715.9668802	12.30
89	02-TricapCubeB----ReC2-----379	-715.9668799	12.30
90	04-Icos-1vx----ReC2-----763	-715.9668600	12.31
91	04-Icos-1vx----ReC2-----793	-715.9668587	12.32
92	03-OhfusetopentBipyr----ReC2-----486	-715.9668349	12.33
93	02-TricapCubeA----ReC2-----253	-715.9656962	13.04
94	02-TricapCubeA----ReC2-----191	-715.9656950	13.05
95	02-TricapCubeB----ReC2-----406	-715.9656660	13.06
96	02-TricapCubeB----ReC2-----382	-715.9656628	13.07
97	04-Icos-1vx----ReC2-----936	-715.9656524	13.07
98	04-Icos-1vx----ReC2-----977	-715.9656524	13.07
99	02-TricapCubeB----ReC2-----384	-715.9656515	13.07
100	02-TricapCubeB----ReC2-----370	-715.9656440	13.08
101	02-TricapCubeB----ReC2-----417	-715.9656440	13.08
102	02-TricapCubeB----ReC2-----328	-715.9656423	13.08
103	02-TricapCubeB----ReC2-----327	-715.9656395	13.08
104	02-TricapCubeB----ReC2-----350	-715.9656385	13.08
105	02-TricapCubeB----ReC2-----314	-715.9656118	13.10
106	02-TricapCubeB----ReC2-----361	-715.9656118	13.10
107	02-TricapCubeB----ReC2-----369	-715.9656085	13.10
108	04-Icos-1vx----ReC2-----863	-715.9655941	13.11

109	02-TricapCubeB----ReC2-----313	-715.9655905	13.11
110	02-TricapCubeB----ReC2-----260	-715.9655859	13.11
111	02-TricapCubeB----ReC2-----312	-715.9655834	13.12
112	04-Icos-1vx----ReC2-----720	-715.9655782	13.12
113	04-Icos-1vx----ReC2-----768	-715.9644482	13.83
114	04-Icos-1vx----ReC2-----745	-715.9644410	13.83
115	02-TricapCubeB----ReC2-----365_i-29	-715.9641238	14.03
116	02-TricapCubeB----ReC2-----323_i-28	-715.9641190	14.03
117	02-TricapCubeB----ReC2-----378_i-25	-715.9640434	14.08
118	04-Icos-1vx----ReC2-----718	-715.9605172	16.29
119	04-Icos-1vx----ReC2-----875	-715.9603768	16.38
120	04-Icos-1vx----ReC2-----715	-715.9603265	16.41
121	02-TricapCubeA----ReC2-----210	-715.9588482	17.34
122	02-TricapCubeA----ReC2-----233	-715.9588482	17.34
123	03-OhfusettoPentBipyr----ReC2-----563	-715.9588375	17.35
124	04-Icos-1vx----ReC2-----790	-715.9563748	18.89
125	04-Icos-1vx----ReC2-----803	-715.9563748	18.89
126	04-Icos-1vx----ReC2-----919	-715.9561936	19.01
127	03-OhfusettoPentBipyr----ReC2-----577_r-34	-715.9542535	20.23
128	03-OhfusettoPentBipyr----ReC2-----569	-715.9541972	20.26
129	03-OhfusettoPentBipyr----ReC2-----543	-715.9529786	21.03
130	01-PentaCapTrPr----ReC2-----2	-715.9529734	21.03
131	03-OhfusettoPentBipyr----ReC2-----686	-715.9527840	21.15
132	03-OhfusettoPentBipyr----ReC2-----515	-715.9527691	21.16
133	04-Icos-1vx----ReC2-----762	-715.9527545	21.17
134	04-Icos-1vx----ReC2-----785	-715.9527545	21.17
135	02-TricapCubeA----ReC2-----187	-715.9527511	21.17
136	02-TricapCubeA----ReC2-----236	-715.9527511	21.17

137	02-TricapCubeB----ReC2-----300	-715.9527434	21.17
138	04-Icos-1vx----ReC2-----925	-715.9527373	21.18
139	04-Icos-1vx----ReC2-----945	-715.9527053	21.20
140	02-TricapCubeB----ReC2-----280	-715.9522821	21.46
141	04-Icos-1vx----ReC2-----982	-715.9522656	21.47
142	03-OhfusettoPentBipyr----ReC2-----532	-715.9522143	21.50
143	02-TricapCubeA----ReC2-----222	-715.9522118	21.51
144	02-TricapCubeA----ReC2-----232	-715.9522072	21.51
145	04-Icos-1vx----ReC2-----755	-715.9522042	21.51
146	04-Icos-1vx----ReC2-----788	-715.9522042	21.51
147	03-OhfusettoPentBipyr----ReC2-----497	-715.9520489	21.61
148	01-PentaCapTrPr----ReC2-----75	-715.9520434	21.61
149	03-OhfusettoPentBipyr----ReC2-----498	-715.9520030	21.64
150	03-OhfusettoPentBipyr----ReC2-----511	-715.9520030	21.64
151	03-OhfusettoPentBipyr----ReC2-----518	-715.9520019	21.64
152	03-OhfusettoPentBipyr----ReC2-----524	-715.9519380	21.68
153	02-TricapCubeA----ReC2-----248	-715.9510828	22.21
154	02-TricapCubeA----ReC2-----223	-715.9510825	22.22
155	02-TricapCubeA----ReC2-----227	-715.9503913	22.65
156	02-TricapCubeA----ReC2-----237	-715.9503913	22.65
157	02-TricapCubeB----ReC2-----271	-715.9503702	22.66
158	01-PentaCapTrPr----ReC2-----14	-715.9503575	22.67
159	01-PentaCapTrPr----ReC2-----5	-715.9503575	22.67
160	01-PentaCapTrPr----ReC2-----27	-715.9503522	22.67
161	01-PentaCapTrPr----ReC2-----47	-715.9503522	22.67
162	02-TricapCubeA----ReC2-----242	-715.9502771	22.72
163	02-TricapCubeA----ReC2-----206	-715.9502770	22.72
164	02-TricapCubeB----ReC2-----275	-715.9502394	22.74

165	04-Icos-1vx---ReC2-----744	-715.9498433	22.99
166	01-PentaCapTrPr---ReC2-----6	-715.9498241	23.00
167	01-PentaCapTrPr---ReC2-----54	-715.9497111	23.08
168	02-TricapCubeB---ReC2-----358	-715.9480128	24.14
169	02-TricapCubeB---ReC2-----388	-715.9479767	24.16
170	02-TricapCubeB---ReC2-----415	-715.9479767	24.16
171	01-PentaCapTrPr---ReC2-----28	-715.9479576	24.18
172	03-OhfusetopentBipyr---ReC2---577_i-34	-715.9479436	24.18
173	03-OhfusetopentBipyr---ReC2-----661	-715.9479014	24.21
174	02-TricapCubeA---ReC2-----90	-715.9478999	24.21
175	04-Icos-1vx---ReC2-----728	-715.9477112	24.33
176	02-TricapCubeA---ReC2-----107	-715.9458850	25.48
177	02-TricapCubeB---ReC2-----270	-715.9455155	25.71
178	02-TricapCubeB---ReC2-----291	-715.9455155	25.71
179	02-TricapCubeB---ReC2-----289	-715.9455054	25.71
180	02-TricapCubeB---ReC2-----302	-715.9455054	25.71
181	02-TricapCubeA---ReC2-----256	-715.9454876	25.73
182	02-TricapCubeA---ReC2-----224	-715.9454869	25.73
183	02-TricapCubeB---ReC2-----273	-715.9452906	25.85
184	02-TricapCubeA---ReC2-----238	-715.9450250	26.02
185	02-TricapCubeA---ReC2-----243	-715.9450250	26.02
186	02-TricapCubeB---ReC2-----368	-715.9449468	26.07
187	02-TricapCubeB---ReC2-----346	-715.9449213	26.08
188	02-TricapCubeB---ReC2-----424	-715.9449181	26.08
189	02-TricapCubeB---ReC2-----259	-715.9449165	26.08
190	04-Icos-1vx---ReC2-----930	-715.9449103	26.09
191	02-TricapCubeB---ReC2-----272	-715.9449019	26.09
192	02-TricapCubeB---ReC2-----402	-715.9448763	26.11

193	02-TricapCubeB----ReC2-----321_i-11	-715.9443670	26.43
194	02-TricapCubeB----ReC2-----317_i-11	-715.9443660	26.43
195	02-TricapCubeB----ReC2-----321_r-11	-715.9443303	26.45
196	02-TricapCubeB----ReC2-----317_r-11	-715.9443297	26.45
197	02-TricapCubeB----ReC2-----373	-715.9442905	26.48
198	02-TricapCubeB----ReC2-----377	-715.9442905	26.48
199	03-OhfusettoPentBipyr----ReC2-----530	-715.9442664	26.49
200	03-OhfusettoPentBipyr----ReC2-----540	-715.9442632	26.49
201	04-Icos-1vx----ReC2-----857	-715.9442593	26.50
202	04-Icos-1vx----ReC2-----865	-715.9442593	26.50
203	02-TricapCubeA----ReC2-----133	-715.9442421	26.51
204	04-Icos-1vx----ReC2-----760	-715.9442349	26.51
205	04-Icos-1vx----ReC2-----749	-715.9442321	26.51
206	04-Icos-1vx----ReC2-----717	-715.9442268	26.52
207	02-TricapCubeB----ReC2-----306	-715.9441057	26.59
208	04-Icos-1vx----ReC2-----974	-715.9432361	27.14
209	04-Icos-1vx----ReC2-----949	-715.9429663	27.31
210	02-TricapCubeB----ReC2-----267	-715.9429589	27.31
211	02-TricapCubeB----ReC2-----307	-715.9429531	27.32
212	01-PentaCapTrPr----ReC2-----45	-715.9429485	27.32
213	01-PentaCapTrPr----ReC2-----51	-715.9429479	27.32
214	04-Icos-1vx----ReC2-----963	-715.9429439	27.32
215	04-Icos-1vx----ReC2-----947	-715.9429330	27.33
216	02-TricapCubeB----ReC2-----355	-715.9429300	27.33
217	02-TricapCubeB----ReC2-----364	-715.9429253	27.33
218	03-OhfusettoPentBipyr----ReC2-----625	-715.9429175	27.34
219	03-OhfusettoPentBipyr----ReC2-----635	-715.9429175	27.34
220	03-OhfusettoPentBipyr----ReC2-----674	-715.9429156	27.34

221	04-Icos-1vx---ReC2-----748	-715.9429084	27.34
222	04-Icos-1vx---ReC2-----800	-715.9429084	27.34
223	04-Icos-1vx---ReC2-----831	-715.9429052	27.35
224	02-TricapCubeB---ReC2-----326	-715.9424865	27.61
225	02-TricapCubeB---ReC2-----334	-715.9424863	27.61
226	02-TricapCubeB---ReC2-----383	-715.9424577	27.63
227	02-TricapCubeB---ReC2-----390	-715.9424577	27.63
228	02-TricapCubeB---ReC2-----304	-715.9417998	28.04
229	02-TricapCubeB---ReC2-----257	-715.9417992	28.04
230	02-TricapCubeA---ReC2-----99	-715.9417834	28.05
231	02-TricapCubeB---ReC2-----279	-715.9415343	28.21
232	02-TricapCubeA---ReC2-----215	-715.9410999	28.48
233	02-TricapCubeA---ReC2-----249	-715.9410995	28.48
234	02-TricapCubeB---ReC2-----362	-715.9410653	28.50
235	04-Icos-1vx---ReC2-----957	-715.9409720	28.56
236	02-TricapCubeB---ReC2-----288	-715.9409712	28.56
237	02-TricapCubeB---ReC2-----262	-715.9409602	28.57
238	04-Icos-1vx---ReC2-----771	-715.9404538	28.88
239	04-Icos-1vx---ReC2-----794	-715.9404538	28.88
240	02-TricapCubeB---ReC2-----340	-715.9403468	28.95
241	02-TricapCubeB---ReC2-----356	-715.9403457	28.95
242	02-TricapCubeB---ReC2-----352	-715.9402058	29.04
243	02-TricapCubeB---ReC2-----408	-715.9401728	29.06
244	04-Icos-1vx---ReC2-----780	-715.9401680	29.06
245	04-Icos-1vx---ReC2-----783	-715.9401480	29.08
246	04-Icos-1vx---ReC2-----774	-715.9397342	29.34
247	04-Icos-1vx---ReC2-----802	-715.9397342	29.34
248	04-Icos-1vx---ReC2-----961	-715.9396239	29.41

249	02-TricapCubeB----ReC2-----416	-715.9396144	29.41
250	02-TricapCubeA----ReC2-----195	-715.9395988	29.42
251	02-TricapCubeA----ReC2-----140	-715.9386708	30.00
252	02-TricapCubeA----ReC2-----235	-715.9386159	30.04
253	03-OhfusettoPentBipyr----ReC2-----679	-715.9385889	30.06
254	03-OhfusettoPentBipyr----ReC2-----697	-715.9385882	30.06
255	04-Icos-1vx----ReC2-----867_r-32	-715.9385744	30.06
256	02-TricapCubeB----ReC2-----396	-715.9385444	30.08
257	02-TricapCubeB----ReC2-----412	-715.9385444	30.08
258	02-TricapCubeB----ReC2-----277	-715.9384138	30.16
259	04-Icos-1vx----ReC2-----759	-715.9382073	30.29
260	04-Icos-1vx----ReC2-----813	-715.9382073	30.29
261	02-TricapCubeB----ReC2-----316	-715.9373632	30.82
262	02-TricapCubeB----ReC2-----353	-715.9373632	30.82
263	02-TricapCubeB----ReC2-----371	-715.9373269	30.85
264	02-TricapCubeB----ReC2-----409	-715.9373269	30.85
265	03-OhfusettoPentBipyr----ReC2-----613	-715.9369654	31.07
266	03-OhfusettoPentBipyr----ReC2-----484	-715.9364877	31.37
267	04-Icos-1vx----ReC2-----714	-715.9363779	31.44
268	04-Icos-1vx----ReC2-----879	-715.9363740	31.44
269	04-Icos-1vx----ReC2-----877	-715.9363674	31.45
270	02-TricapCubeA----ReC2-----91	-715.9363456	31.46
271	02-TricapCubeB----ReC2-----295	-715.9363432	31.46
272	04-Icos-1vx----ReC2-----844	-715.9363337	31.47
273	01-PentaCapTrPr----ReC2-----60	-715.9363141	31.48
274	02-TricapCubeB----ReC2-----430	-715.9362994	31.49
275	04-Icos-1vx----ReC2-----731	-715.9362188	31.54
276	01-PentaCapTrPr----ReC2-----22	-715.9361790	31.57

277	01-PentaCapTrPr----ReC2-----56	-715.9361747	31.57
278	04-Icos-1vx----ReC2-----918	-715.9358594	31.77
279	01-PentaCapTrPr----ReC2-----70	-715.9345472	32.59
280	03-OhfusetopentBipyr----ReC2-----575	-715.9345432	32.59
281	03-OhfusetopentBipyr----ReC2-----522	-715.9345352	32.60
282	03-OhfusetopentBipyr----ReC2-----509	-715.9345302	32.60
283	04-Icos-1vx----ReC2-----825	-715.9344940	32.62
284	04-Icos-1vx----ReC2-----861	-715.9344913	32.63
285	03-OhfusetopentBipyr----ReC2-----560	-715.9344857	32.63
286	03-OhfusetopentBipyr----ReC2-----579	-715.9344849	32.63
287	03-OhfusetopentBipyr----ReC2-----529	-715.9344085	32.68
288	04-Icos-1vx----ReC2-----864	-715.9338802	33.01
289	02-TricapCubeA----ReC2-----251	-715.9333374	33.35
290	02-TricapCubeA----ReC2-----239	-715.9333370	33.35
291	01-PentaCapTrPr----ReC2-----21	-715.9333342	33.35
292	01-PentaCapTrPr----ReC2-----16	-715.9333281	33.36
293	02-TricapCubeB----ReC2-----411	-715.9333233	33.36
294	02-TricapCubeB----ReC2-----419	-715.9333233	33.36
295	04-Icos-1vx----ReC2-----787	-715.9333105	33.37
296	04-Icos-1vx----ReC2-----795	-715.9333105	33.37
297	04-Icos-1vx----ReC2-----895	-715.9332937	33.38
298	04-Icos-1vx----ReC2-----754	-715.9328955	33.63
299	04-Icos-1vx----ReC2-----772	-715.9328955	33.63
300	02-TricapCubeA----ReC2-----252	-715.9313384	34.60
301	04-Icos-1vx----ReC2-----791	-715.9312591	34.65
302	04-Icos-1vx----ReC2-----811	-715.9312591	34.65
303	03-OhfusetopentBipyr----ReC2-----580	-715.9304981	35.13
304	01-PentaCapTrPr----ReC2-----12	-715.9304598	35.16

305	03-OhfusettoPentBipyr----ReC2-----513	-715.9304041	35.19
306	04-Icos-1vx----ReC2-----867_i-32	-715.9303006	35.26
307	04-Icos-1vx----ReC2-----779	-715.9300742	35.40
308	02-TricapCubeB----ReC2-----342	-715.9285139	36.38
309	02-TricapCubeB----ReC2-----332	-715.9285113	36.38
310	01-PentaCapTrPr----ReC2-----18	-715.9284845	36.40
311	02-TricapCubeA----ReC2-----244	-715.9284379	36.43
312	04-Icos-1vx----ReC2-----807	-715.9284140	36.44
313	04-Icos-1vx----ReC2-----815	-715.9284140	36.44
314	03-OhfusettoPentBipyr----ReC2-----690	-715.9270545	37.29
315	02-TricapCubeB----ReC2-----285	-715.9270543	37.29
316	02-TricapCubeB----ReC2-----278	-715.9270285	37.31
317	04-Icos-1vx----ReC2-----874	-715.9268287	37.43
318	02-TricapCubeA----ReC2-----212	-715.9267891	37.46
319	02-TricapCubeA----ReC2-----185	-715.9267890	37.46
320	02-TricapCubeB----ReC2-----268	-715.9267426	37.49
321	04-Icos-1vx----ReC2-----733	-715.9267265	37.50
322	04-Icos-1vx----ReC2-----756	-715.9267028	37.51
323	04-Icos-1vx----ReC2-----796	-715.9267028	37.51
324	02-TricapCubeA----ReC2-----255	-715.9266980	37.52
325	02-TricapCubeB----ReC2-----366	-715.9266921	37.52
326	02-TricapCubeA----ReC2-----247	-715.9266907	37.52
327	02-TricapCubeB----ReC2-----331	-715.9266905	37.52
328	02-TricapCubeB----ReC2-----387	-715.9266687	37.54
329	02-TricapCubeB----ReC2-----423	-715.9266651	37.54
330	02-TricapCubeA----ReC2-----234	-715.9261273	37.87
331	02-TricapCubeA----ReC2-----202	-715.9261236	37.88
332	04-Icos-1vx----ReC2-----934	-715.9260936	37.90

333	04-Icos-1vx---ReC2-----969	-715.9260936	37.90
334	02-TricapCubeB---ReC2-----359	-715.9260924	37.90
335	02-TricapCubeB---ReC2-----349	-715.9260877	37.90
336	02-TricapCubeB---ReC2-----404	-715.9260540	37.92
337	02-TricapCubeB---ReC2-----414	-715.9260507	37.92
338	03-OhfusettoPentBipyr---ReC2-----572	-715.9253392	38.37
339	02-TricapCubeA---ReC2-----220	-715.9248077	38.70
340	02-TricapCubeB---ReC2-----381	-715.9248045	38.71
341	02-TricapCubeB---ReC2-----397	-715.9248045	38.71
342	04-Icos-1vx---ReC2-----960	-715.9247738	38.72
343	04-Icos-1vx---ReC2-----978	-715.9247738	38.72
344	03-OhfusettoPentBipyr---ReC2-----545	-715.9247613	38.73
345	02-TricapCubeB---ReC2-----324	-715.9247530	38.74
346	02-TricapCubeB---ReC2-----341	-715.9247521	38.74
347	02-TricapCubeB---ReC2-----284	-715.9247483	38.74
348	02-TricapCubeB---ReC2-----309	-715.9247474	38.74
349	03-OhfusettoPentBipyr---ReC2-----510	-715.9236270	39.44
350	03-OhfusettoPentBipyr---ReC2-----521	-715.9235206	39.51
351	02-TricapCubeB---ReC2-----258	-715.9233159	39.64
352	02-TricapCubeB---ReC2-----320	-715.9233120	39.64
353	02-TricapCubeB---ReC2-----374	-715.9232782	39.66
354	02-TricapCubeB---ReC2-----401	-715.9232772	39.66
355	02-TricapCubeB---ReC2-----319	-715.9232401	39.69
356	02-TricapCubeB---ReC2-----345	-715.9232401	39.69
357	04-Icos-1vx---ReC2-----859	-715.9232210	39.70
358	04-Icos-1vx---ReC2-----950	-715.9232161	39.70
359	04-Icos-1vx---ReC2-----971	-715.9232161	39.70
360	04-Icos-1vx---ReC2-----830	-715.9232116	39.70

361	04-Icos-1vx---ReC2-----846	-715.9232065	39.71
362	02-TricapCubeB---ReC2-----376	-715.9232022	39.71
363	02-TricapCubeA---ReC2-----108	-715.9231741	39.73
364	01-PentaCapTrPr---ReC2-----87	-715.9229784	39.85
365	02-TricapCubeA---ReC2-----131	-715.9229527	39.87
366	02-TricapCubeA---ReC2-----178	-715.9229522	39.87
367	03-OhfusetopentBipyr---ReC2-----578	-715.9227205	40.01
368	02-TricapCubeA---ReC2-----190	-715.9225863	40.10
369	02-TricapCubeA---ReC2-----245	-715.9225845	40.10
370	03-OhfusetopentBipyr---ReC2-----600	-715.9223697	40.23
371	03-OhfusetopentBipyr---ReC2-----616	-715.9223681	40.23
372	04-Icos-1vx---ReC2-----833	-715.9223005	40.28
373	01-PentaCapTrPr---ReC2-----9	-715.9213584	40.87
374	01-PentaCapTrPr---ReC2-----36	-715.9213575	40.87
375	03-OhfusetopentBipyr---ReC2-----587	-715.9207873	41.23
376	03-OhfusetopentBipyr---ReC2-----621	-715.9207873	41.23
377	04-Icos-1vx---ReC2-----753	-715.9207741	41.23
378	04-Icos-1vx---ReC2-----764	-715.9207741	41.23
379	01-PentaCapTrPr---ReC2-----37	-715.9206120	41.34
380	01-PentaCapTrPr---ReC2-----49	-715.9206120	41.34
381	02-TricapCubeA---ReC2-----217	-715.9205617	41.37
382	02-TricapCubeA---ReC2-----216	-715.9205574	41.37
383	04-Icos-1vx---ReC2-----716	-715.9203629	41.49
384	04-Icos-1vx---ReC2-----738	-715.9203629	41.49
385	03-OhfusetopentBipyr---ReC2-----559	-715.9203601	41.49
386	03-OhfusetopentBipyr---ReC2-----544	-715.9203084	41.53
387	01-PentaCapTrPr---ReC2-----82	-715.9200063	41.72
388	02-TricapCubeA---ReC2-----100	-715.9195884	41.98

389	04-Icos-1vx---ReC2-----750	-715.9195747	41.99
390	04-Icos-1vx---ReC2-----824	-715.9195747	41.99
391	02-TricapCubeB---ReC2-----446	-715.9195395	42.01
392	02-TricapCubeB---ReC2-----330	-715.9191730	42.24
393	02-TricapCubeB---ReC2-----363	-715.9190782	42.30
394	02-TricapCubeB---ReC2-----339	-715.9190773	42.30
395	04-Icos-1vx---ReC2-----798	-715.9189346	42.39
396	04-Icos-1vx---ReC2-----804	-715.9189346	42.39
397	03-OhfusettoPentBipyr---ReC2-----542	-715.9186631	42.56
398	03-OhfusettoPentBipyr---ReC2-----570	-715.9186631	42.56
399	01-PentaCapTrPr---ReC2-----58	-715.9186305	42.58
400	02-TricapCubeA---ReC2-----161	-715.9186221	42.58
401	03-OhfusettoPentBipyr---ReC2-----489	-715.9185107	42.65
402	03-OhfusettoPentBipyr---ReC2-----490	-715.9184763	42.68
403	03-OhfusettoPentBipyr---ReC2-----624	-715.9183013	42.79
404	03-OhfusettoPentBipyr---ReC2-----611	-715.9183000	42.79
405	02-TricapCubeA---ReC2-----130	-715.9182886	42.79
406	02-TricapCubeA---ReC2-----138	-715.9182869	42.79
407	02-TricapCubeB---ReC2-----471	-715.9182708	42.81
408	02-TricapCubeA---ReC2-----219	-715.9181614	42.87
409	02-TricapCubeA---ReC2-----240	-715.9181609	42.87
410	01-PentaCapTrPr---ReC2-----1	-715.9181147	42.90
411	01-PentaCapTrPr---ReC2-----38	-715.9181121	42.90
412	03-OhfusettoPentBipyr---ReC2-----582	-715.9180699	42.93
413	03-OhfusettoPentBipyr---ReC2-----552	-715.9180687	42.93
414	04-Icos-1vx---ReC2-----852	-715.9180429	42.95
415	01-PentaCapTrPr---ReC2-----84	-715.9180299	42.96
416	02-TricapCubeA---ReC2-----201	-715.9179977	42.98

417	02-TricapCubeA----ReC2-----209	-715.9179977	42.98
418	04-Icos-1vx----ReC2-----832	-715.9179920	42.98
419	04-Icos-1vx----ReC2-----782	-715.9179811	42.99
420	04-Icos-1vx----ReC2-----940	-715.9178118	43.09
421	04-Icos-1vx----ReC2-----777	-715.9172991	43.41
422	04-Icos-1vx----ReC2-----956	-715.9170116	43.60
423	02-TricapCubeB----ReC2-----301	-715.9169835	43.61
424	04-Icos-1vx----ReC2-----839	-715.9169524	43.63
425	02-TricapCubeA----ReC2-----96	-715.9164576	43.94
426	04-Icos-1vx----ReC2-----781	-715.9164412	43.95
427	04-Icos-1vx----ReC2-----873	-715.9163806	43.99
428	04-Icos-1vx----ReC2-----836	-715.9156717	44.44
429	02-TricapCubeA----ReC2-----150	-715.9156380	44.46
430	02-TricapCubeA----ReC2-----166	-715.9156378	44.46
431	02-TricapCubeA----ReC2-----169	-715.9156347	44.46
432	02-TricapCubeA----ReC2-----119	-715.9155857	44.49
433	03-OhfusettoPentBipyr----ReC2-----473	-715.9153457	44.64
434	03-OhfusettoPentBipyr----ReC2-----500	-715.9153422	44.64
435	04-Icos-1vx----ReC2-----730	-715.9153395	44.64
436	02-TricapCubeA----ReC2-----95	-715.9153091	44.66
437	03-OhfusettoPentBipyr----ReC2-----646	-715.9152859	44.68
438	03-OhfusettoPentBipyr----ReC2-----602	-715.9152803	44.68
439	03-OhfusettoPentBipyr----ReC2-----691	-715.9152792	44.68
440	03-OhfusettoPentBipyr----ReC2-----651	-715.9152781	44.68
441	01-PentaCapTrPr----ReC2-----68	-715.9152721	44.69
442	03-OhfusettoPentBipyr----ReC2-----519	-715.9152717	44.69
443	03-OhfusettoPentBipyr----ReC2-----499	-715.9152679	44.69
444	02-TricapCubeB----ReC2-----425	-715.9152141	44.72

445	02-TricapCubeB----ReC2-----437	-715.9152141	44.72
446	01-PentaCapTrPr----ReC2-----85	-715.9152138	44.72
447	02-TricapCubeA----ReC2-----173	-715.9151895	44.74
448	02-TricapCubeB----ReC2-----436	-715.9149165	44.91
449	02-TricapCubeB----ReC2-----457	-715.9149165	44.91
450	04-Icos-1vx----ReC2-----866	-715.9149139	44.91
451	02-TricapCubeA----ReC2-----103	-715.9149129	44.91
452	03-OhfusetopentBipyr----ReC2-----609	-715.9148974	44.92
453	03-OhfusetopentBipyr----ReC2-----640	-715.9148953	44.92
454	04-Icos-1vx----ReC2-----944	-715.9148810	44.93
455	02-TricapCubeA----ReC2-----167	-715.9148706	44.94
456	02-TricapCubeA----ReC2-----151	-715.9148634	44.94
457	02-TricapCubeA----ReC2-----153	-715.9148616	44.94
458	04-Icos-1vx----ReC2-----799	-715.9147166	45.04
459	04-Icos-1vx----ReC2-----812	-715.9147166	45.04
460	02-TricapCubeB----ReC2-----281	-715.9145447	45.14
461	04-Icos-1vx----ReC2-----902	-715.9144757	45.19
462	04-Icos-1vx----ReC2-----915	-715.9144757	45.19
463	04-Icos-1vx----ReC2-----900	-715.9144639	45.19
464	02-TricapCubeA----ReC2-----125	-715.9143723	45.25
465	02-TricapCubeB----ReC2-----428	-715.9143515	45.26
466	02-TricapCubeB----ReC2-----453	-715.9143515	45.26
467	02-TricapCubeB----ReC2-----290	-715.9143489	45.27
468	02-TricapCubeB----ReC2-----308	-715.9143438	45.27
469	02-TricapCubeA----ReC2-----112	-715.9143204	45.28
470	02-TricapCubeA----ReC2-----189	-715.9141182	45.41
471	02-TricapCubeA----ReC2-----229	-715.9141182	45.41
472	04-Icos-1vx----ReC2-----734	-715.9140761	45.44

473	02-TricapCubeB----ReC2-----305	-715.9137946	45.61
474	04-Icos-1vx----ReC2-----723	-715.9137479	45.64
475	04-Icos-1vx----ReC2-----828	-715.9137042	45.67
476	02-TricapCubeB----ReC2-----426	-715.9136609	45.70
477	03-OhfusettoPentBipyr----ReC2-----620	-715.9135260	45.78
478	02-TricapCubeB----ReC2-----431	-715.9134226	45.85
479	02-TricapCubeB----ReC2-----470	-715.9134226	45.85
480	03-OhfusettoPentBipyr----ReC2-----696	-715.9133936	45.87
481	03-OhfusettoPentBipyr----ReC2-----684	-715.9133913	45.87
482	04-Icos-1vx----ReC2-----851	-715.9133778	45.88
483	02-TricapCubeA----ReC2-----170	-715.9133648	45.88
484	02-TricapCubeA----ReC2-----111	-715.9133569	45.89
485	02-TricapCubeA----ReC2-----213	-715.9133169	45.91
486	02-TricapCubeA----ReC2-----225	-715.9133169	45.91
487	02-TricapCubeA----ReC2-----179	-715.9131959	45.99
488	04-Icos-1vx----ReC2-----840	-715.9131953	45.99
489	02-TricapCubeA----ReC2-----139	-715.9131952	45.99
490	03-OhfusettoPentBipyr----ReC2-----576	-715.9131624	46.01
491	03-OhfusettoPentBipyr----ReC2-----583	-715.9131609	46.01
492	03-OhfusettoPentBipyr----ReC2-----514	-715.9131051	46.05
493	03-OhfusettoPentBipyr----ReC2-----506	-715.9131023	46.05
494	02-TricapCubeA----ReC2-----104	-715.9130947	46.05
495	04-Icos-1vx----ReC2-----739	-715.9130746	46.07
496	01-PentaCapTrPr----ReC2-----57	-715.9130609	46.07
497	01-PentaCapTrPr----ReC2-----81	-715.9130609	46.07
498	02-TricapCubeB----ReC2-----432	-715.9130147	46.10
499	04-Icos-1vx----ReC2-----823	-715.9129978	46.11
500	04-Icos-1vx----ReC2-----757	-715.9128458	46.21

501	04-Icos-1vx---ReC2-----821	-715.9128458	46.21
502	04-Icos-1vx---ReC2-----896	-715.9125859	46.37
503	04-Icos-1vx---ReC2-----922	-715.9125859	46.37
504	04-Icos-1vx---ReC2-----941	-715.9125732	46.38
505	04-Icos-1vx---ReC2-----872	-715.9125726	46.38
506	04-Icos-1vx---ReC2-----761	-715.9122621	46.58
507	04-Icos-1vx---ReC2-----769	-715.9122621	46.58
508	01-PentaCapTrPr---ReC2-----69	-715.9119353	46.78
509	02-TricapCubeA---ReC2-----89	-715.9119125	46.80
510	01-PentaCapTrPr---ReC2-----4	-715.9118983	46.80
511	03-OhfusetopentBipyr---ReC2-----505	-715.9118118	46.86
512	04-Icos-1vx---ReC2-----871_i-17	-715.9117592	46.89
513	04-Icos-1vx---ReC2-----871_r-17	-715.9116413	46.97
514	04-Icos-1vx---ReC2-----843	-715.9113643	47.14
515	02-TricapCubeB---ReC2-----462	-715.9113207	47.17
516	04-Icos-1vx---ReC2-----948	-715.9112967	47.18
517	03-OhfusetopentBipyr---ReC2-----547	-715.9112722	47.20
518	03-OhfusetopentBipyr---ReC2-----557	-715.9112717	47.20
519	03-OhfusetopentBipyr---ReC2-----555	-715.9112659	47.20
520	04-Icos-1vx---ReC2-----892	-715.9112327	47.22
521	04-Icos-1vx---ReC2-----894	-715.9111891	47.25
522	04-Icos-1vx---ReC2-----914	-715.9111891	47.25
523	04-Icos-1vx---ReC2-----906	-715.9102528	47.84
524	04-Icos-1vx---ReC2-----891	-715.9102484	47.84
525	04-Icos-1vx---ReC2-----893	-715.9102307	47.85
526	04-Icos-1vx---ReC2-----911	-715.9102264	47.85
527	02-TricapCubeA---ReC2-----157	-715.9100221	47.98
528	02-TricapCubeB---ReC2-----443	-715.9100179	47.98

529	02-TricapCubeB----ReC2-----451	-715.9100179	47.98
530	04-Icos-1vx----ReC2-----819	-715.9099742	48.01
531	04-Icos-1vx----ReC2-----789	-715.9099732	48.01
532	04-Icos-1vx----ReC2-----928	-715.9098968	48.06
533	02-TricapCubeA----ReC2-----211	-715.9095218	48.30
534	02-TricapCubeB----ReC2-----380	-715.9094958	48.31
535	02-TricapCubeB----ReC2-----413	-715.9094952	48.31
536	02-TricapCubeB----ReC2-----325	-715.9094723	48.33
537	02-TricapCubeB----ReC2-----357	-715.9094711	48.33
538	02-TricapCubeA----ReC2-----218	-715.9094656	48.33
539	02-TricapCubeA----ReC2-----208	-715.9094624	48.33
540	02-TricapCubeB----ReC2-----389	-715.9093567	48.40
541	02-TricapCubeB----ReC2-----399	-715.9093540	48.40
542	04-Icos-1vx----ReC2-----773	-715.9093015	48.43
543	04-Icos-1vx----ReC2-----818	-715.9093015	48.43
544	04-Icos-1vx----ReC2-----937	-715.9092202	48.48
545	02-TricapCubeB----ReC2-----422	-715.9091836	48.51
546	02-TricapCubeB----ReC2-----403	-715.9091823	48.51
547	02-TricapCubeB----ReC2-----274	-715.9091736	48.51
548	02-TricapCubeB----ReC2-----347	-715.9091587	48.52
549	02-TricapCubeB----ReC2-----367	-715.9091587	48.52
550	02-TricapCubeA----ReC2-----171	-715.9091098	48.55
551	02-TricapCubeA----ReC2-----142	-715.9091096	48.55
552	04-Icos-1vx----ReC2-----778	-715.9089933	48.63
553	02-TricapCubeA----ReC2-----115	-715.9088407	48.72
554	02-TricapCubeA----ReC2-----192	-715.9085940	48.88
555	02-TricapCubeA----ReC2-----221	-715.9085940	48.88
556	02-TricapCubeB----ReC2-----329	-715.9085893	48.88

557	02-TricapCubeB----ReC2-----318	-715.9085864	48.88
558	02-TricapCubeB----ReC2-----375	-715.9085130	48.93
559	02-TricapCubeB----ReC2-----385	-715.9085130	48.93
560	04-Icos-1vx----ReC2-----908	-715.9081219	49.17
561	04-Icos-1vx----ReC2-----935	-715.9081206	49.17
562	04-Icos-1vx----ReC2-----917	-715.9080157	49.24
563	02-TricapCubeA----ReC2-----156	-715.9075599	49.53
564	02-TricapCubeA----ReC2-----183	-715.9075546	49.53
565	04-Icos-1vx----ReC2-----814	-715.9072796	49.70
566	04-Icos-1vx----ReC2-----849	-715.9059069	50.56
567	04-Icos-1vx----ReC2-----860	-715.9058650	50.59
568	02-TricapCubeA----ReC2-----105	-715.9058593	50.59
569	02-TricapCubeB----ReC2-----311_i-25	-715.9053974	50.88
570	02-TricapCubeB----ReC2-----311_r-25	-715.9053502	50.91
571	02-TricapCubeB----ReC2-----303	-715.9052142	51.00
572	04-Icos-1vx----ReC2-----899_i-18	-715.9051284	51.05
573	02-TricapCubeB----ReC2-----394	-715.9051254	51.05
574	02-TricapCubeB----ReC2-----395_i-12	-715.9050994	51.07
575	02-TricapCubeB----ReC2-----420_i-12	-715.9050994	51.07
576	04-Icos-1vx----ReC2-----907	-715.9050746	51.09
577	02-TricapCubeB----ReC2-----338	-715.9050605	51.09
578	04-Icos-1vx----ReC2-----899_r-18	-715.9050556	51.10
579	04-Icos-1vx----ReC2-----938	-715.9050508	51.10
580	02-TricapCubeB----ReC2-----395_r-12	-715.9050178	51.12
581	02-TricapCubeB----ReC2-----420_r-12	-715.9050178	51.12
582	04-Icos-1vx----ReC2-----901	-715.9050034	51.13
583	03-OhfusettoPentBipyr----ReC2-----664	-715.9047493	51.29
584	03-OhfusettoPentBipyr----ReC2-----682	-715.9047491	51.29

585	01-PentaCapTrPr----ReC2-----77	-715.9029763	52.40
586	02-TricapCubeB----ReC2-----266	-715.9027293	52.56
587	02-TricapCubeB----ReC2-----297	-715.9026557	52.60
588	03-OhfusetopentBipyr----ReC2-----538	-715.9026458	52.61
589	03-OhfusetopentBipyr----ReC2-----554	-715.9026424	52.61
590	03-OhfusetopentBipyr----ReC2-----526	-715.9019485	53.05
591	03-OhfusetopentBipyr----ReC2-----553	-715.9010348	53.62
592	02-TricapCubeA----ReC2-----197	-715.9007555	53.80
593	03-OhfusetopentBipyr----ReC2-----539	-715.9005897	53.90
594	01-PentaCapTrPr----ReC2-----35	-715.8993676	54.67
595	03-OhfusetopentBipyr----ReC2-----487	-715.8992896	54.72
596	03-OhfusetopentBipyr----ReC2-----501	-715.8992815	54.72
597	04-Icos-1vx----ReC2-----826	-715.8990655	54.86
598	04-Icos-1vx----ReC2-----869	-715.8990637	54.86
599	01-PentaCapTrPr----ReC2-----78	-715.8988209	55.01
600	02-TricapCubeA----ReC2-----143	-715.8988126	55.02
601	02-TricapCubeA----ReC2-----193	-715.8987930	55.03
602	02-TricapCubeA----ReC2-----230	-715.8986868	55.09
603	02-TricapCubeA----ReC2-----246	-715.8986868	55.09
604	04-Icos-1vx----ReC2-----841	-715.8986457	55.12
605	04-Icos-1vx----ReC2-----862	-715.8986434	55.12
606	04-Icos-1vx----ReC2-----719	-715.8986253	55.13
607	04-Icos-1vx----ReC2-----722	-715.8986253	55.13
608	03-OhfusetopentBipyr----ReC2-----565	-715.8985548	55.18
609	01-PentaCapTrPr----ReC2-----23	-715.8974908	55.84
610	01-PentaCapTrPr----ReC2-----8	-715.8974908	55.84
611	02-TricapCubeA----ReC2-----160	-715.8974279	55.88
612	02-TricapCubeA----ReC2-----128	-715.8974204	55.89

613	04-Icos-1vx---ReC2-----806	-715.8971550	56.06
614	04-Icos-1vx---ReC2-----822	-715.8971550	56.06
615	02-TricapCubeA---ReC2-----136	-715.8971449	56.06
616	02-TricapCubeA---ReC2-----122	-715.8971421	56.06
617	02-TricapCubeB---ReC2-----450	-715.8970949	56.09
618	04-Icos-1vx---ReC2-----726	-715.8970822	56.10
619	03-OhfusetopentBipyr---ReC2-----592	-715.8970736	56.11
620	03-OhfusetopentBipyr---ReC2-----614	-715.8970600	56.12
621	03-OhfusetopentBipyr---ReC2-----517	-715.8968165	56.27
622	03-OhfusetopentBipyr---ReC2-----523	-715.8968140	56.27
623	01-PentacappedTriprism---ReC2-----67	-715.8967762	56.29
624	01-PentacappedTriprism---ReC2-----15	-715.8967421	56.31
625	01-PentacappedTriprism---ReC2-----29	-715.8967421	56.31
626	02-TricapCubeA---ReC2-----181	-715.8962835	56.60
627	04-Icos-1vx---ReC2-----741	-715.8961434	56.69
628	02-TricapCubeB---ReC2-----456	-715.8961072	56.71
629	02-TricapCubeA---ReC2-----120	-715.8959469	56.81
630	02-TricapCubeB---ReC2-----454	-715.8958610	56.87
631	04-Icos-1vx---ReC2-----747	-715.8958225	56.89
632	04-Icos-1vx---ReC2-----792	-715.8958221	56.89
633	02-TricapCubeA---ReC2-----231	-715.8958202	56.89
634	02-TricapCubeA---ReC2-----254	-715.8958202	56.89
635	02-TricapCubeA---ReC2-----97	-715.8954522	57.12
636	04-Icos-1vx---ReC2-----724	-715.8954336	57.14
637	02-TricapCubeB---ReC2-----442	-715.8954171	57.15
638	04-Icos-1vx---ReC2-----909	-715.8951312	57.33
639	02-TricapCubeB---ReC2-----386	-715.8951015	57.34
640	02-TricapCubeA---ReC2-----141	-715.8949163	57.46

641	04-Icos-1vx---ReC2-----727	-715.8949117	57.46
642	02-TricapCubeB---ReC2-----466	-715.8948893	57.48
643	04-Icos-1vx---ReC2-----713	-715.8948192	57.52
644	04-Icos-1vx---ReC2-----729	-715.8948192	57.52
645	04-Icos-1vx---ReC2-----910	-715.8948053	57.53
646	04-Icos-1vx---ReC2-----916	-715.8948053	57.53
647	02-TricapCubeA---ReC2-----154	-715.8948030	57.53
648	02-TricapCubeA---ReC2-----135	-715.8947982	57.53
649	04-Icos-1vx---ReC2-----842	-715.8947926	57.54
650	04-Icos-1vx---ReC2-----870	-715.8947926	57.54
651	03-OhfusettoPentBipyr---ReC2-----641	-715.8947864	57.54
652	03-OhfusettoPentBipyr---ReC2-----633	-715.8947849	57.54
653	03-OhfusettoPentBipyr---ReC2-----599	-715.8947606	57.56
654	03-OhfusettoPentBipyr---ReC2-----607	-715.8947582	57.56
655	02-TricapCubeB---ReC2-----438	-715.8947032	57.59
656	03-OhfusettoPentBipyr---ReC2-----677	-715.8938354	58.14
657	04-Icos-1vx---ReC2-----968	-715.8925232	58.96
658	04-Icos-1vx---ReC2-----980	-715.8925232	58.96
659	02-TricapCubeA---ReC2-----106	-715.8924763	58.99
660	03-OhfusettoPentBipyr---ReC2-----650	-715.8924637	59.00
661	03-OhfusettoPentBipyr---ReC2-----658	-715.8924602	59.00
662	04-Icos-1vx---ReC2-----837_i-122	-715.8924249	59.02
663	04-Icos-1vx---ReC2-----837_r-122	-715.8922275	59.15
664	04-Icos-1vx---ReC2-----981	-715.8920063	59.29
665	04-Icos-1vx---ReC2-----758	-715.8915555	59.57
666	04-Icos-1vx---ReC2-----805	-715.8915555	59.57
667	01-PentaCapTrPr---ReC2-----42	-715.8913882	59.67
668	02-TricapCubeB---ReC2-----464	-715.8911759	59.81

669	02-TricapCubeB----ReC2-----434	-715.8911235	59.84
670	02-TricapCubeB----ReC2-----441	-715.8911235	59.84
671	04-Icos-1vx----ReC2-----765	-715.8909909	59.92
672	04-Icos-1vx----ReC2-----817	-715.8909909	59.92
673	02-TricapCubeB----ReC2-----458	-715.8904396	60.27
674	04-Icos-1vx----ReC2-----766	-715.8903527	60.32
675	04-Icos-1vx----ReC2-----801	-715.8903527	60.32
676	02-TricapCubeA----ReC2-----198	-715.8900795	60.50
677	04-Icos-1vx----ReC2-----975	-715.8900286	60.53
678	02-TricapCubeA----ReC2-----200	-715.8900245	60.53
679	04-Icos-1vx----ReC2-----973	-715.8899171	60.60
680	04-Icos-1vx----ReC2-----965	-715.8896968	60.74
681	02-TricapCubeB----ReC2-----293	-715.8893130	60.98
682	04-Icos-1vx----ReC2-----838	-715.8886341	61.40
683	01-PentaCapTrPr----ReC2-----72	-715.8885496	61.46
684	01-PentaCapTrPr----ReC2-----79	-715.8885496	61.46
685	02-TricapCubeA----ReC2-----165	-715.8885234	61.47
686	02-TricapCubeA----ReC2-----149	-715.8885226	61.47
687	04-Icos-1vx----ReC2-----933	-715.8883230	61.60
688	02-TricapCubeA----ReC2-----164	-715.8876294	62.03
689	02-TricapCubeA----ReC2-----148	-715.8876232	62.04
690	02-TricapCubeA----ReC2-----186	-715.8875884	62.06
691	02-TricapCubeA----ReC2-----204	-715.8875884	62.06
692	02-TricapCubeA----ReC2-----92	-715.8875396	62.09
693	02-TricapCubeA----ReC2-----93	-715.8874883	62.12
694	02-TricapCubeA----ReC2-----98	-715.8874883	62.12
695	02-TricapCubeA----ReC2-----180	-715.8874869	62.12
696	01-PentaCapTrPr----ReC2-----64	-715.8874841	62.12

697	01-PentaCapTrPr----ReC2-----73	-715.8874841	62.12
698	02-TricapCubeA----ReC2-----116	-715.8874815	62.13
699	02-TricapCubeB----ReC2-----427	-715.8874293	62.16
700	02-TricapCubeB----ReC2-----445	-715.8874293	62.16
701	02-TricapCubeA----ReC2-----109	-715.8873703	62.20
702	04-Icos-1vx----ReC2-----912	-715.8873310	62.22
703	04-Icos-1vx----ReC2-----924	-715.8873310	62.22
704	02-TricapCubeA----ReC2-----205	-715.8872492	62.27
705	02-TricapCubeA----ReC2-----226	-715.8872492	62.27
706	04-Icos-1vx----ReC2-----827	-715.8869962	62.43
707	04-Icos-1vx----ReC2-----858	-715.8866094	62.67
708	03-OhfusettoPentBipyr----ReC2-----537	-715.8865886	62.69
709	03-OhfusettoPentBipyr----ReC2-----496	-715.8865784	62.69
710	01-PentaCapTrPr----ReC2-----76	-715.8865189	62.73
711	02-TricapCubeA----ReC2-----228	-715.8862411	62.90
712	03-OhfusettoPentBipyr----ReC2-----503	-715.8860182	63.04
713	03-OhfusettoPentBipyr----ReC2-----502	-715.8860180	63.04
714	03-OhfusettoPentBipyr----ReC2-----527	-715.8860165	63.05
715	02-TricapCubeB----ReC2-----292	-715.8858448	63.15
716	02-TricapCubeB----ReC2-----310	-715.8858403	63.16
717	02-TricapCubeB----ReC2-----429	-715.8858371	63.16
718	02-TricapCubeB----ReC2-----461	-715.8858371	63.16
719	02-TricapCubeA----ReC2-----113	-715.8855667	63.33
720	04-Icos-1vx----ReC2-----854	-715.8853489	63.46
721	04-Icos-1vx----ReC2-----845	-715.8853478	63.46
722	04-Icos-1vx----ReC2-----984	-715.8853128	63.49
723	04-Icos-1vx----ReC2-----856_r-17	-715.8850640	63.64
724	04-Icos-1vx----ReC2-----856_i-17	-715.8850449	63.66

725	04-Icos-1vx---ReC2-----964	-715.8843793	64.07
726	02-TricapCubeA---ReC2-----124	-715.8843358	64.10
727	02-TricapCubeA---ReC2-----184	-715.8843355	64.10
728	04-Icos-1vx---ReC2-----931	-715.8843288	64.10
729	01-PentaCapTrPr---ReC2-----50	-715.8841975	64.19
730	04-Icos-1vx---ReC2-----890	-715.8841839	64.20
731	04-Icos-1vx---ReC2-----898	-715.8841829	64.20
732	04-Icos-1vx---ReC2-----904	-715.8841211	64.23
733	04-Icos-1vx---ReC2-----923	-715.8841211	64.23
734	04-Icos-1vx---ReC2-----903	-715.8840958	64.25
735	04-Icos-1vx---ReC2-----881	-715.8840395	64.29
736	04-Icos-1vx---ReC2-----889	-715.8840395	64.29
737	03-OhfusettoPentBipyr---ReC2-----665	-715.8838465	64.41
738	03-OhfusettoPentBipyr---ReC2-----676	-715.8838465	64.41
739	01-PentaCapTrPr---ReC2-----80	-715.8829886	64.95
740	03-OhfusettoPentBipyr---ReC2-----675	-715.8827206	65.11
741	03-OhfusettoPentBipyr---ReC2-----689	-715.8827187	65.11
742	02-TricapCubeB---ReC2-----449	-715.8826450	65.16
743	02-TricapCubeB---ReC2-----435	-715.8826389	65.16
744	01-PentaCapTrPr---ReC2-----26	-715.8823542	65.34
745	02-TricapCubeB---ReC2-----264	-715.8821938	65.44
746	04-Icos-1vx---ReC2-----847	-715.8815064	65.88
747	01-PentaCapTrPr---ReC2-----48	-715.8810954	66.13
748	02-TricapCubeB---ReC2-----452	-715.8796245	67.06
749	02-TricapCubeB---ReC2-----460	-715.8796245	67.06
750	02-TricapCubeB---ReC2-----294	-715.8796193	67.06
751	02-TricapCubeB---ReC2-----286	-715.8796140	67.06
752	02-TricapCubeA---ReC2-----121	-715.8796113	67.06

753	02-TricapCubeA----ReC2-----152	-715.8796113	67.06
754	02-TricapCubeA----ReC2-----168	-715.8796113	67.06
755	03-OhfusetopentBipyr----ReC2-----657	-715.8795774	67.09
756	03-OhfusetopentBipyr----ReC2-----673	-715.8795774	67.09
757	04-Icos-1vx----ReC2-----955	-715.8790775	67.40
758	04-Icos-1vx----ReC2-----962	-715.8790775	67.40
759	04-Icos-1vx----ReC2-----952	-715.8778514	68.17
760	04-Icos-1vx----ReC2-----979	-715.8778514	68.17
761	02-TricapCubeA----ReC2-----110	-715.8778079	68.20
762	03-OhfusetopentBipyr----ReC2-----660	-715.8778046	68.20
763	03-OhfusetopentBipyr----ReC2-----666	-715.8778031	68.20
764	04-Icos-1vx----ReC2-----967	-715.8769960	68.71
765	03-OhfusetopentBipyr----ReC2-----615	-715.8765019	69.02
766	04-Icos-1vx----ReC2-----834	-715.8764939	69.02
767	03-OhfusetopentBipyr----ReC2-----474	-715.8759965	69.33
768	03-OhfusetopentBipyr----ReC2-----512	-715.8759965	69.33
769	03-OhfusetopentBipyr----ReC2-----693	-715.8758198	69.44
770	03-OhfusetopentBipyr----ReC2-----603	-715.8757492	69.49
771	03-OhfusetopentBipyr----ReC2-----622	-715.8757492	69.49
772	03-OhfusetopentBipyr----ReC2-----568	-715.8755787	69.60
773	03-OhfusetopentBipyr----ReC2-----692	-715.8755451	69.62
774	01-PentaCapTrPr----ReC2-----63	-715.8749654	69.98
775	01-PentaCapTrPr----ReC2-----20	-715.8745078	70.27
776	03-OhfusetopentBipyr----ReC2-----481	-715.8744794	70.29
777	03-OhfusetopentBipyr----ReC2-----482	-715.8744506	70.30
778	03-OhfusetopentBipyr----ReC2-----508	-715.8744505	70.30
779	03-OhfusetopentBipyr----ReC2-----567	-715.8743576	70.36
780	01-PentaCapTrPr----ReC2-----10	-715.8740311	70.57

781	02-TricapCubeA----ReC2-----174	-715.8736778	70.79
782	04-Icos-1vx----ReC2-----725	-715.8736513	70.80
783	04-Icos-1vx----ReC2-----743	-715.8736513	70.80
784	04-Icos-1vx----ReC2-----932	-715.8730057	71.21
785	04-Icos-1vx----ReC2-----721	-715.8722920	71.66
786	04-Icos-1vx----ReC2-----735	-715.8722920	71.66
787	02-TricapCubeA----ReC2-----158	-715.8722832	71.66
788	02-TricapCubeB----ReC2-----433	-715.8722273	71.70
789	01-PentaCapTrPr----ReC2-----66	-715.8722127	71.71
790	01-PentaCapTrPr----ReC2-----86	-715.8722127	71.71
791	02-TricapCubeB----ReC2-----472	-715.8716373	72.07
792	04-Icos-1vx----ReC2-----742	-715.8716279	72.07
793	02-TricapCubeB----ReC2-----455	-715.8715810	72.10
794	02-TricapCubeB----ReC2-----468	-715.8715810	72.10
795	02-TricapCubeA----ReC2-----123	-715.8715720	72.11
796	02-TricapCubeA----ReC2-----144	-715.8715720	72.11
797	03-OhfusettoPentBipyr----ReC2-----595	-715.8706078	72.71
798	03-OhfusettoPentBipyr----ReC2-----623	-715.8706078	72.71
799	03-OhfusettoPentBipyr----ReC2-----659	-715.8701399	73.01
800	03-OhfusettoPentBipyr----ReC2-----644	-715.8699644	73.12
801	02-TricapCubeB----ReC2-----298	-715.8699513	73.13
802	03-OhfusettoPentBipyr----ReC2-----593	-715.8696953	73.29
803	03-OhfusettoPentBipyr----ReC2-----639	-715.8696947	73.29
804	04-Icos-1vx----ReC2-----966	-715.8695743	73.36
805	04-Icos-1vx----ReC2-----972	-715.8695743	73.36
806	02-TricapCubeB----ReC2-----265	-715.8695312	73.39
807	04-Icos-1vx----ReC2-----951	-715.8693270	73.52
808	02-TricapCubeB----ReC2-----444	-715.8693079	73.53

809	02-TricapCubeB----ReC2-----459	-715.8693079	73.53
810	02-TricapCubeB----ReC2-----440	-715.8688669	73.81
811	04-Icos-1vx----ReC2-----732	-715.8688591	73.81
812	04-Icos-1vx----ReC2-----737	-715.8688591	73.81
813	02-TricapCubeA----ReC2-----114	-715.8684746	74.05
814	04-Icos-1vx----ReC2-----868	-715.8682463	74.20
815	04-Icos-1vx----ReC2-----850	-715.8682461	74.20
816	02-TricapCubeA----ReC2-----101	-715.8682267	74.21
817	02-TricapCubeA----ReC2-----194	-715.8677689	74.50
818	04-Icos-1vx----ReC2-----959	-715.8676221	74.59
819	02-TricapCubeA----ReC2-----129	-715.8675408	74.64
820	04-Icos-1vx----ReC2-----740	-715.8672852	74.80
821	02-TricapCubeB----ReC2-----448	-715.8672259	74.84
822	03-OhfusettoPentBipyr----ReC2-----548	-715.8672246	74.84
823	03-OhfusettoPentBipyr----ReC2-----627	-715.8669914	74.98
824	03-OhfusettoPentBipyr----ReC2-----619	-715.8669730	75.00
825	03-OhfusettoPentBipyr----ReC2-----495	-715.8669705	75.00
826	02-TricapCubeB----ReC2-----439	-715.8669664	75.00
827	02-TricapCubeB----ReC2-----465	-715.8669664	75.00
828	03-OhfusettoPentBipyr----ReC2-----494	-715.8669542	75.01
829	01-PentaCapTrPr----ReC2-----30	-715.8668996	75.04
830	01-PentaCapTrPr----ReC2-----24	-715.8668780	75.06
831	01-PentaCapTrPr----ReC2-----32	-715.8668780	75.06
832	01-PentaCapTrPr----ReC2-----55	-715.8667975	75.11
833	03-OhfusettoPentBipyr----ReC2-----566	-715.8665798	75.24
834	02-TricapCubeB----ReC2-----447	-715.8663135	75.41
835	02-TricapCubeB----ReC2-----467	-715.8663135	75.41
836	02-TricapCubeA----ReC2-----177	-715.8662130	75.47

837	02-TricapCubeA----ReC2-----147	-715.8662096	75.47
838	02-TricapCubeA----ReC2-----163	-715.8662082	75.48
839	02-TricapCubeB----ReC2-----463	-715.8654905	75.93
840	02-TricapCubeB----ReC2-----469	-715.8654905	75.93
841	02-TricapCubeA----ReC2-----127	-715.8642400	76.71
842	02-TricapCubeA----ReC2-----176	-715.8642375	76.71
843	02-TricapCubeA----ReC2-----146	-715.8639959	76.86
844	02-TricapCubeA----ReC2-----162	-715.8639959	76.86
845	02-TricapCubeA----ReC2-----137	-715.8639935	76.87
846	03-OhfusetopentBipyr----ReC2-----493	-715.8635265	77.16
847	01-PentacappedTriprism----ReC2-----59	-715.8632451	77.33
848	04-Icosahedron-1vx----ReC2-----848	-715.8630363	77.47
849	04-Icosahedron-1vx----ReC2-----946	-715.8630184	77.48
850	04-Icosahedron-1vx----ReC2-----954	-715.8630184	77.48
851	04-Icosahedron-1vx----ReC2-----887	-715.8615231	78.42
852	04-Icosahedron-1vx----ReC2-----888	-715.8614549	78.46
853	04-Icosahedron-1vx----ReC2-----921	-715.8614549	78.46
854	01-PentacappedTriprism----ReC2-----34	-715.8614081	78.49
855	01-PentacappedTriprism----ReC2-----41	-715.8614081	78.49
856	04-Icosahedron-1vx----ReC2-----835	-715.8606654	78.95
857	02-TricapCubeA----ReC2-----126	-715.8600830	79.32
858	02-TricapCubeA----ReC2-----145	-715.8599997	79.37
859	03-OhfusetopentBipyr----ReC2-----668	-715.8597821	79.51
860	03-OhfusetopentBipyr----ReC2-----584	-715.8596368	79.60
861	01-PentacappedTriprism----ReC2-----11	-715.8595951	79.63
862	01-PentacappedTriprism----ReC2-----44	-715.8595951	79.63
863	03-OhfusetopentBipyr----ReC2-----610	-715.8595521	79.65
864	03-OhfusetopentBipyr----ReC2-----648	-715.8595521	79.65

865	02-TricapCubeA----ReC2-----117	-715.8595284	79.67
866	04-Icos-1vx----ReC2-----876	-715.8588918	80.07
867	04-Icos-1vx----ReC2-----926	-715.8585712	80.27
868	04-Icos-1vx----ReC2-----920	-715.8584660	80.33
869	04-Icos-1vx----ReC2-----927	-715.8584660	80.33
870	04-Icos-1vx----ReC2-----886	-715.8576754	80.83
871	04-Icos-1vx----ReC2-----913	-715.8576754	80.83
872	04-Icos-1vx----ReC2-----884	-715.8576022	80.88
873	03-OhfusetopentBipyr----ReC2-----479	-715.8562659	81.71
874	03-OhfusetopentBipyr----ReC2-----528	-715.8562000	81.76
875	03-OhfusetopentBipyr----ReC2-----478	-715.8561929	81.76
876	01-PentaCapTrPr----ReC2-----61	-715.8558023	82.01
877	02-TricapCubeA----ReC2-----132	-715.8557562	82.03
878	04-Icos-1vx----ReC2-----829	-715.8556180	82.12
879	04-Icos-1vx----ReC2-----853	-715.8556180	82.12
880	03-OhfusetopentBipyr----ReC2-----597	-715.8555997	82.13
881	04-Icos-1vx----ReC2-----885	-715.8535452	83.42
882	04-Icos-1vx----ReC2-----883	-715.8534721	83.47
883	04-Icos-1vx----ReC2-----905	-715.8534721	83.47
884	04-Icos-1vx----ReC2-----882	-715.8534673	83.47
885	04-Icos-1vx----ReC2-----897	-715.8534673	83.47
886	02-TricapCubeA----ReC2-----102	-715.8512327	84.87
887	03-OhfusetopentBipyr----ReC2-----475	-715.8508403	85.12
888	03-OhfusetopentBipyr----ReC2-----520	-715.8508364	85.12
889	03-OhfusetopentBipyr----ReC2-----476	-715.8508023	85.14
890	04-Icos-1vx----ReC2-----976	-715.8503600	85.42
891	04-Icos-1vx----ReC2-----983	-715.8503600	85.42
892	01-PentaCapTrPr----ReC2-----71	-715.8502330	85.50

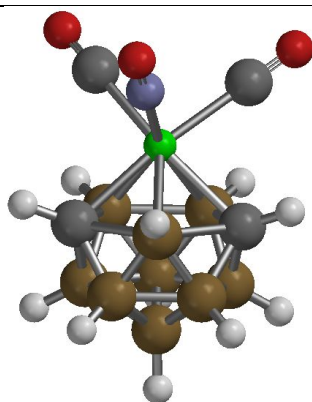
893	04-Icos-1vx---ReC2-----855	-715.8499158	85.70
894	02-TricapCubeA---ReC2-----182	-715.8498873	85.72
895	02-TricapCubeA---ReC2-----172	-715.8498789	85.72
896	03-OhfusettoPentBipyr---ReC2-----581	-715.8491513	86.18
897	03-OhfusettoPentBipyr---ReC2-----536	-715.8490849	86.22
898	02-TricapCubeB---ReC2-----299	-715.8440597	89.37
899	01-PentaCapTrPr---ReC2-----25	-715.8428642	90.12
900	01-PentaCapTrPr---ReC2-----39	-715.8428642	90.12
901	03-OhfusettoPentBipyr---ReC2-----534	-715.8426667	90.25
902	03-OhfusettoPentBipyr---ReC2-----573	-715.8426667	90.25
903	03-OhfusettoPentBipyr---ReC2-----535	-715.8416415	90.89
904	03-OhfusettoPentBipyr---ReC2-----601	-715.8415126	90.97
905	03-OhfusettoPentBipyr---ReC2-----638	-715.8415126	90.97
906	01-PentaCapTrPr---ReC2-----62	-715.8413139	91.10
907	01-PentaCapTrPr---ReC2-----65	-715.8413139	91.10
908	02-TricapCubeA---ReC2-----175	-715.8403862	91.68
909	02-TricapCubeA---ReC2-----159	-715.8403786	91.68
910	03-OhfusettoPentBipyr---ReC2-----507	-715.8394233	92.28
911	03-OhfusettoPentBipyr---ReC2-----550	-715.8381768	93.07
912	03-OhfusettoPentBipyr---ReC2-----574	-715.8381768	93.07
913	03-OhfusettoPentBipyr---ReC2-----492	-715.8367439	93.96
914	03-OhfusettoPentBipyr---ReC2-----491	-715.8367327	93.97
915	03-OhfusettoPentBipyr---ReC2-----551	-715.8358629	94.52
916	03-OhfusettoPentBipyr---ReC2-----590	-715.8333822	96.07
917	02-TricapCubeA---ReC2-----155	-715.8324459	96.66
918	03-OhfusettoPentBipyr---ReC2-----618	-715.8324009	96.69
919	03-OhfusettoPentBipyr---ReC2-----642	-715.8324009	96.69
920	03-OhfusettoPentBipyr---ReC2-----480	-715.8315662	97.21

921	03-OhfusetopentBipyr----ReC2-----504	-715.8315662	97.21
922	03-OhfusetopentBipyr----ReC2-----711	-715.8305277	97.87
923	01-PentaCapTrPr----ReC2-----17	-715.8298448	98.29
924	01-PentaCapTrPr----ReC2-----40	-715.8298448	98.29
925	03-OhfusetopentBipyr----ReC2-----667	-715.8279100	99.51
926	03-OhfusetopentBipyr----ReC2-----652	-715.8279096	99.51
927	03-OhfusetopentBipyr----ReC2-----680	-715.8271541	99.98
928	03-OhfusetopentBipyr----ReC2-----681	-715.8271541	99.98
929	03-OhfusetopentBipyr----ReC2-----698	-715.8268339	100.18
930	03-OhfusetopentBipyr----ReC2-----663	-715.8268244	100.19
931	01-PentaCapTrPr----ReC2-----3	-715.8241362	101.88
932	01-PentaCapTrPr----ReC2-----46	-715.8241362	101.88
933	03-OhfusetopentBipyr----ReC2-----647	-715.8184110	105.47
934	03-OhfusetopentBipyr----ReC2-----594	-715.8184101	105.47
935	03-OhfusetopentBipyr----ReC2-----558	-715.8182866	105.55
936	03-OhfusetopentBipyr----ReC2-----571	-715.8182866	105.55
937	01-PentaCapTrPr----ReC2-----74	-715.8177885	105.86
938	01-PentaCapTrPr----ReC2-----88	-715.8177885	105.86
939	03-OhfusetopentBipyr----ReC2-----628	-715.8169431	106.39
940	03-OhfusetopentBipyr----ReC2-----533	-715.8105783	110.38
941	03-OhfusetopentBipyr----ReC2-----549	-715.8105783	110.38
942	03-OhfusetopentBipyr----ReC2-----702	-715.8080020	112.00
943	01-PentaCapTrPr----ReC2-----33	-715.8076211	112.24
944	03-OhfusetopentBipyr----ReC2-----488	-715.8065801	112.89
945	03-OhfusetopentBipyr----ReC2-----477	-715.8065732	112.90
946	03-OhfusetopentBipyr----ReC2-----589	-715.8064475	112.98
947	03-OhfusetopentBipyr----ReC2-----541	-715.8064196	112.99
948	03-OhfusetopentBipyr----ReC2-----546	-715.8064196	112.99

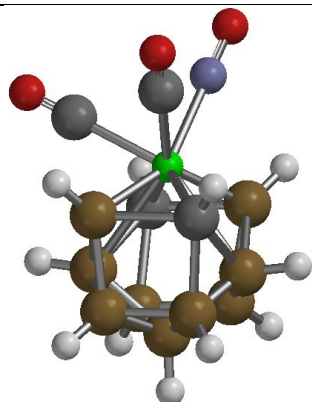
949	03-OhfusetopentBipyr----ReC2-----704	-715.8041647	114.41
950	03-OhfusetopentBipyr----ReC2-----688	-715.8041632	114.41
951	03-OhfusetopentBipyr----ReC2-----671	-715.8033903	114.89
952	03-OhfusetopentBipyr----ReC2-----695	-715.8028443	115.24
953	03-OhfusetopentBipyr----ReC2-----700	-715.7994089	117.39
954	03-OhfusetopentBipyr----ReC2-----678	-715.7970818	118.85
955	03-OhfusetopentBipyr----ReC2-----705	-715.7970817	118.85
956	03-OhfusetopentBipyr----ReC2-----626	-715.7962114	119.40
957	03-OhfusetopentBipyr----ReC2-----643	-715.7962068	119.40
958	03-OhfusetopentBipyr----ReC2-----703	-715.7956930	119.73
959	03-OhfusetopentBipyr----ReC2-----706	-715.7909175	122.72
960	03-OhfusetopentBipyr----ReC2-----662	-715.7909107	122.73
961	03-OhfusetopentBipyr----ReC2-----637	-715.7906773	122.87
962	03-OhfusetopentBipyr----ReC2-----585	-715.7906706	122.88
963	03-OhfusetopentBipyr----ReC2-----701	-715.7893950	123.68
964	03-OhfusetopentBipyr----ReC2-----606	-715.7877359	124.72
965	03-OhfusetopentBipyr----ReC2-----670	-715.7838879	127.13
966	03-OhfusetopentBipyr----ReC2-----709	-715.7838879	127.13
967	03-OhfusetopentBipyr----ReC2-----653	-715.7825026	128.00
968	03-OhfusetopentBipyr----ReC2-----710	-715.7821785	128.21
969	03-OhfusetopentBipyr----ReC2-----617	-715.7795938	129.83
970	03-OhfusetopentBipyr----ReC2-----634	-715.7795938	129.83
971	03-OhfusetopentBipyr----ReC2-----604	-715.7794319	129.93
972	03-OhfusetopentBipyr----ReC2-----630	-715.7794319	129.93
973	03-OhfusetopentBipyr----ReC2-----612	-715.7794022	129.95
974	03-OhfusetopentBipyr----ReC2-----632	-715.7794022	129.95
975	03-OhfusetopentBipyr----ReC2-----654	-715.7789932	130.20
976	03-OhfusetopentBipyr----ReC2-----707	-715.7789932	130.20

977	03-OhfusetopentBipyr----ReC2-----605	-715.7781925	130.71
978	03-OhfusetopentBipyr----ReC2-----687	-715.7763877	131.84
979	03-OhfusetopentBipyr----ReC2-----712	-715.7763753	131.85
980	03-OhfusetopentBipyr----ReC2-----586	-715.7746621	132.92
981	03-OhfusetopentBipyr----ReC2-----645	-715.7746621	132.92
982	03-OhfusetopentBipyr----ReC2-----636	-715.7715187	134.89
983	03-OhfusetopentBipyr----ReC2-----672	-715.7703914	135.60
984	03-OhfusetopentBipyr----ReC2-----685	-715.7703914	135.60
985	03-OhfusetopentBipyr----ReC2-----588	-715.7698165	135.96
986	03-OhfusetopentBipyr----ReC2-----629	-715.7698165	135.96
987	03-OhfusetopentBipyr----ReC2-----591	-715.7691238	136.40
988	03-OhfusetopentBipyr----ReC2-----598	-715.7691238	136.40
989	03-OhfusetopentBipyr----ReC2-----483	-715.7674786	137.43
990	03-OhfusetopentBipyr----ReC2-----516	-715.7674786	137.43
991	03-OhfusetopentBipyr----ReC2-----655	-715.7657359	138.52
992	03-OhfusetopentBipyr----ReC2-----699	-715.7657344	138.52
993	03-OhfusetopentBipyr----ReC2-----596	-715.7641489	139.52
994	03-OhfusetopentBipyr----ReC2-----631	-715.7641489	139.52
995	03-OhfusetopentBipyr----ReC2-----608	-715.7609140	141.55
996	03-OhfusetopentBipyr----ReC2-----669	-715.7476383	149.88
997	03-OhfusetopentBipyr----ReC2-----683	-715.7472127	150.15
998	03-OhfusetopentBipyr----ReC2-----656	-715.7472084	150.15
999	03-OhfusetopentBipyr----ReC2-----694	-715.7462438	150.76
1000	03-OhfusetopentBipyr----ReC2-----708	-715.7462438	150.76
1001	03-OhfusetopentBipyr----ReC2-----649	-715.7196529	167.44

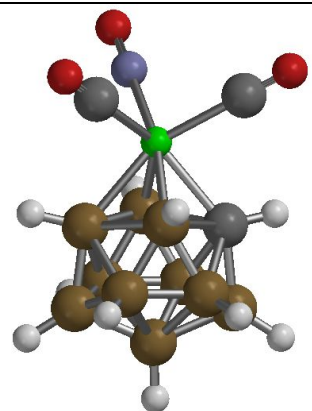
Table 5A. Initial $(\text{CO})_2(\text{NO})\text{ReC}_2\text{B}_9\text{H}_{11}$ structures (one example from each family), a total of 350 structures:



1. Icosahedron 30 structures

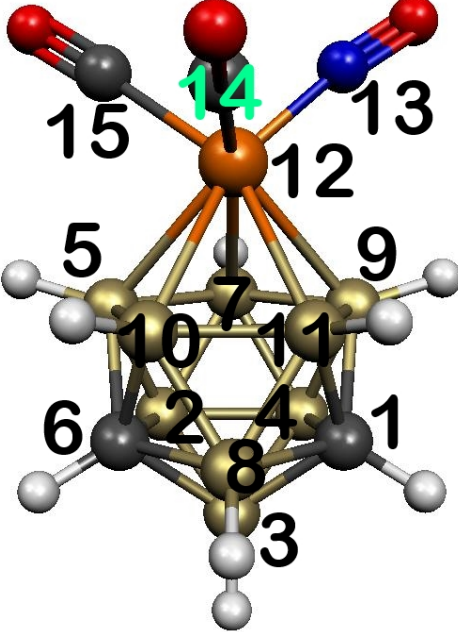


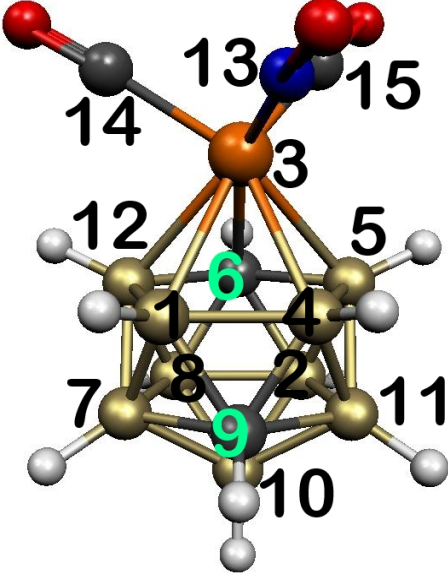
2. Cubeoctahedron 150 structures

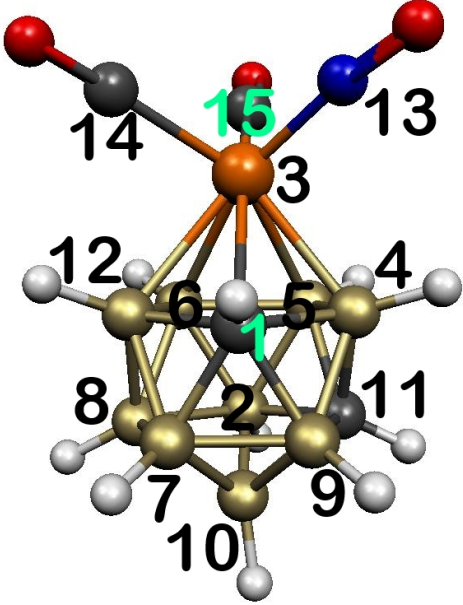


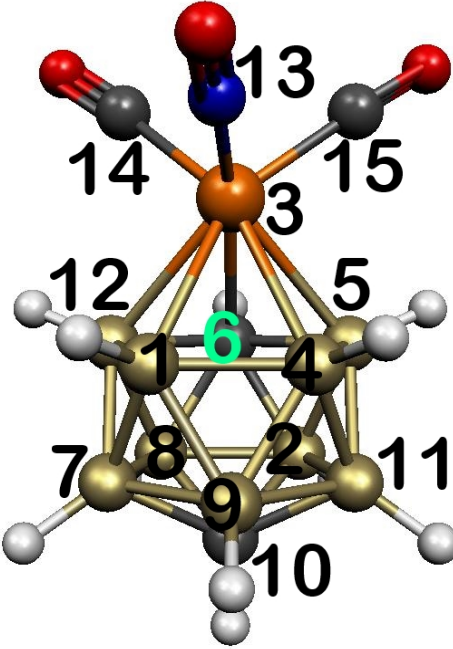
3. Anticubeoctahedron 170 structures

Table 5B. Distances table for the lowest-lying (CO)₂(NO)ReC₂B₉H₁₁ structures after M06L/6-311G(d,p)//SDD optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

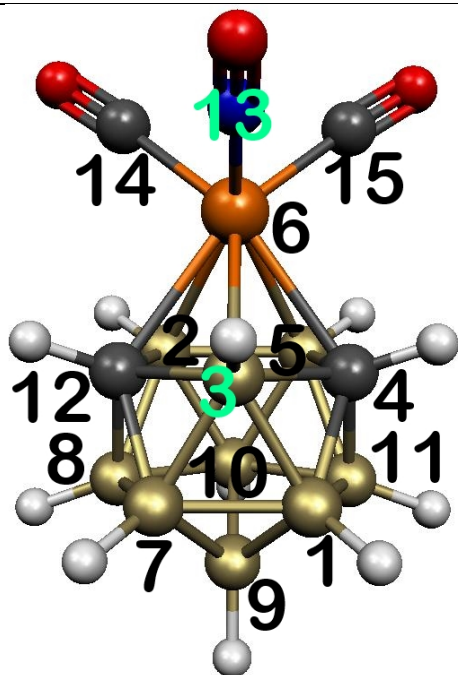
 1. -741.69942670 0.0 (C_s)	1 2 3 4 5				
	1 C	0.000000			
	2 B	2.715735	0.000000		
	3 B	1.672388	1.750248	0.000000	
	4 B	1.683897	1.761201	1.747891	0.000000
	5 B	3.206950	1.756823	2.838802	2.861643
	6 C	2.575723	1.690158	1.673305	2.718384
	7 B	2.747900	1.754377	2.847727	1.760842
	8 B	1.672947	2.847158	1.764553	2.843192
	9 B	1.685941	2.859371	2.839835	1.755278
	10 B	2.740168	2.868806	2.851441	3.380557
	11 B	1.693673	3.388281	2.860208	2.879516
	12 Re	3.433773	3.570773	4.142920	3.562972
	13 N	4.393616	4.865030	5.432789	4.363586
	14 C	4.542109	5.181794	5.386444	5.219818
	15 C	5.168881	4.316894	5.425600	4.903162
		6	7	8	9
	6 C	0.000000			
	7 B	2.748776	0.000000		
	8 B	1.676621	3.375199	0.000000	
	9 B	3.211927	1.806063	2.847414	0.000000
	10 B	1.682137	2.931430	1.746604	2.913728
	11 B	2.744145	2.940959	1.745824	1.806222
	12 Re	3.450536	2.343771	3.537369	2.307101
	13 N	5.111493	3.231836	5.002487	2.837665
	14 C	4.480105	4.263664	4.168958	3.825324

	15 C 4.343655 3.254445 5.017651 4.065436 3.450055
	11 12 13 14 15
	11 B 0.000000
	12 Re 2.309102 0.000000
	13 N 3.458386 1.839560 0.000000
	14 C 2.913473 1.986331 2.854918 0.000000
 2. -741.69660170 +1.8 (Cs)	15 C 4.175670 1.996545 2.849386 2.871214 0.000000
	1 2 3 4 5
	1 B 0.000000
	2 B 3.380265 0.000000
	3 Re 2.339887 3.586706 0.000000
	4 B 1.811829 2.867097 2.312627 0.000000
	5 B 2.908046 1.770155 2.306610 1.789935 0.000000
	6 C 2.784037 1.683918 2.319702 2.782347 1.719538
	7 B 1.750633 2.844243 3.580561 2.867535 3.363555
	8 B 2.876830 1.754052 3.605502 3.380264 2.865887
	9 C 1.681846 2.705779 3.441257 1.679173 2.722124
	10 B 2.862501 1.749801 4.176954 2.861221 2.858899
	11 B 2.875604 1.752313 3.565867 1.760187 1.762079
	12 B 1.787071 2.842808 2.331579 2.884252 2.864009
	13 N 3.195068 5.075884 1.823255 2.872145 3.515034
	14 C 3.299197 5.033136 1.995472 4.099326 4.147648
	15 C 4.274843 4.268857 1.992464 3.797687 2.923368
	6 7 8 9 10
	6 C 0.000000
	7 B 2.722900 0.000000
	8 B 1.679514 1.761227 0.000000
	9 C 3.050212 1.684637 2.711725 0.000000
	10 B 2.718721 1.766050 1.749619 1.685243 0.000000

	<table><tr><td>11 B</td><td>2.731458</td><td>2.850434</td><td>2.842917</td><td>1.681607</td><td>1.760264</td></tr><tr><td>12 B</td><td>1.689968</td><td>1.751186</td><td>1.764715</td><td>2.710186</td><td>2.842490</td></tr><tr><td>13 N</td><td>4.075653</td><td>4.840490</td><td>5.263631</td><td>4.289433</td><td>5.468661</td></tr><tr><td>14 C</td><td>3.443916</td><td>4.345279</td><td>4.428415</td><td>4.821352</td><td>5.458890</td></tr><tr><td>15 C</td><td>3.031721</td><td>5.242029</td><td>4.684243</td><td>5.090026</td><td>5.456768</td></tr><tr><td></td><td>11</td><td>12</td><td>13</td><td>14</td><td>15</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>3.344425</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>13 N</td><td>4.522952</td><td>3.923601</td><td>0.000000</td><td></td><td></td></tr><tr><td>14 C</td><td>5.321456</td><td>2.785565</td><td>2.811089</td><td>0.000000</td><td></td></tr><tr><td>15 C</td><td>4.642275</td><td>3.812248</td><td>2.810819</td><td>2.869263</td><td>0.000000</td></tr></table>	11 B	2.731458	2.850434	2.842917	1.681607	1.760264	12 B	1.689968	1.751186	1.764715	2.710186	2.842490	13 N	4.075653	4.840490	5.263631	4.289433	5.468661	14 C	3.443916	4.345279	4.428415	4.821352	5.458890	15 C	3.031721	5.242029	4.684243	5.090026	5.456768		11	12	13	14	15	11 B	0.000000					12 B	3.344425	0.000000				13 N	4.522952	3.923601	0.000000			14 C	5.321456	2.785565	2.811089	0.000000		15 C	4.642275	3.812248	2.810819	2.869263	0.000000																																										
11 B	2.731458	2.850434	2.842917	1.681607	1.760264																																																																																																								
12 B	1.689968	1.751186	1.764715	2.710186	2.842490																																																																																																								
13 N	4.075653	4.840490	5.263631	4.289433	5.468661																																																																																																								
14 C	3.443916	4.345279	4.428415	4.821352	5.458890																																																																																																								
15 C	3.031721	5.242029	4.684243	5.090026	5.456768																																																																																																								
	11	12	13	14	15																																																																																																								
11 B	0.000000																																																																																																												
12 B	3.344425	0.000000																																																																																																											
13 N	4.522952	3.923601	0.000000																																																																																																										
14 C	5.321456	2.785565	2.811089	0.000000																																																																																																									
15 C	4.642275	3.812248	2.810819	2.869263	0.000000																																																																																																								
 3. -741.69521340 +2.6 C₁	<table><tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.225036</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Re</td><td>2.325325</td><td>3.569532</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.703380</td><td>2.842351</td><td>2.285921</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.806704</td><td>1.760395</td><td>2.317334</td><td>1.789818</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.803007</td><td>1.760566</td><td>2.341631</td><td>2.883245</td><td>1.807539</td></tr><tr><td>7 B</td><td>1.680815</td><td>2.847667</td><td>3.600732</td><td>2.845532</td><td>3.391406</td></tr><tr><td>8 B</td><td>2.749569</td><td>1.760959</td><td>3.599434</td><td>3.350714</td><td>2.882189</td></tr><tr><td>9 B</td><td>1.671030</td><td>2.834740</td><td>3.573776</td><td>1.760036</td><td>2.874556</td></tr><tr><td>10 B</td><td>2.732186</td><td>1.757010</td><td>4.179539</td><td>2.850718</td><td>2.871251</td></tr><tr><td>11 C</td><td>2.598430</td><td>1.685523</td><td>3.437533</td><td>1.673891</td><td>1.691203</td></tr><tr><td>12 B</td><td>1.704270</td><td>2.836960</td><td>2.329930</td><td>2.833458</td><td>2.882989</td></tr><tr><td>13 N</td><td>3.243377</td><td>5.067330</td><td>1.840024</td><td>2.861825</td><td>3.526282</td></tr><tr><td>14 C</td><td>3.374820</td><td>5.012827</td><td>2.001050</td><td>4.088454</td><td>4.157399</td></tr><tr><td>15 C</td><td>4.216300</td><td>4.236722</td><td>1.972696</td><td>3.756829</td><td>2.903582</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></table>		1	2	3	4	5	1 C	0.000000					2 B	3.225036	0.000000				3 Re	2.325325	3.569532	0.000000			4 B	1.703380	2.842351	2.285921	0.000000		5 B	2.806704	1.760395	2.317334	1.789818	0.000000	6 B	2.803007	1.760566	2.341631	2.883245	1.807539	7 B	1.680815	2.847667	3.600732	2.845532	3.391406	8 B	2.749569	1.760959	3.599434	3.350714	2.882189	9 B	1.671030	2.834740	3.573776	1.760036	2.874556	10 B	2.732186	1.757010	4.179539	2.850718	2.871251	11 C	2.598430	1.685523	3.437533	1.673891	1.691203	12 B	1.704270	2.836960	2.329930	2.833458	2.882989	13 N	3.243377	5.067330	1.840024	2.861825	3.526282	14 C	3.374820	5.012827	2.001050	4.088454	4.157399	15 C	4.216300	4.236722	1.972696	3.756829	2.903582		6	7	8	9	10	6 B	0.000000				
	1	2	3	4	5																																																																																																								
1 C	0.000000																																																																																																												
2 B	3.225036	0.000000																																																																																																											
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14 C	3.374820	5.012827	2.001050	4.088454	4.157399																																																																																																								
15 C	4.216300	4.236722	1.972696	3.756829	2.903582																																																																																																								
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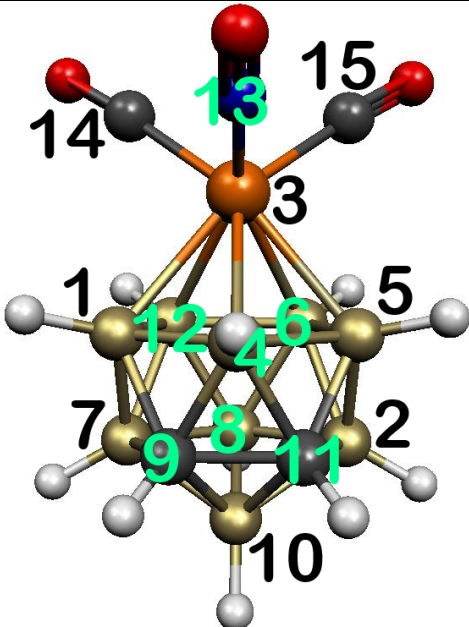
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	10 C 2.731137 1.673164 4.019236 2.730235 2.719390				
	11 B 2.873481 1.750425 3.583016 1.756891 1.756155				
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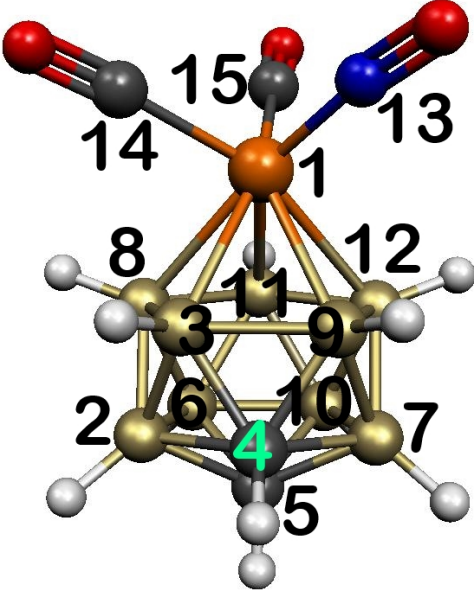
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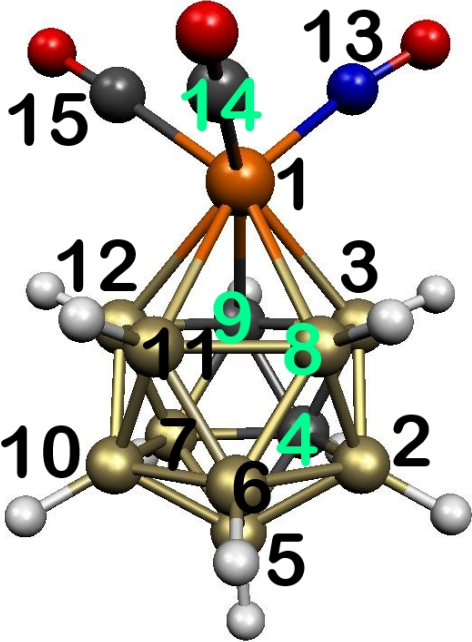


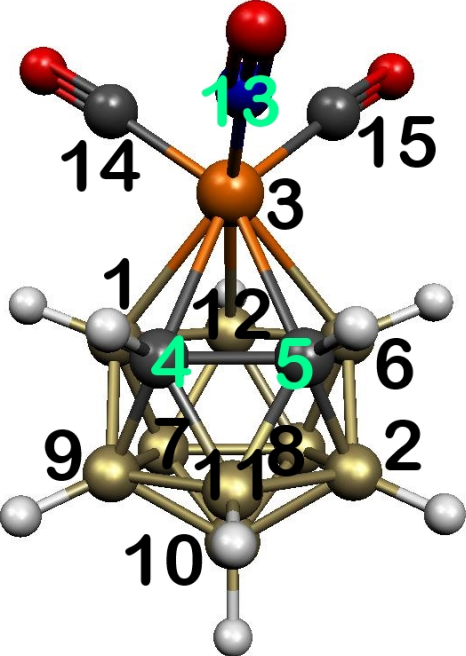
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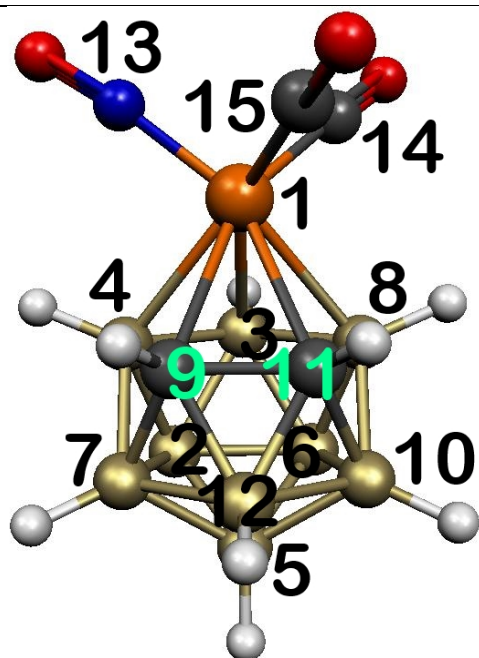
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3 B	2.346941	1.775341	0.000000		
4 B	2.316527	1.761671	1.785029	0.000000	
5 B	4.219518	1.763935	2.884338	2.861688	0.000000
6 B	3.602811	1.763498	1.767578	2.847240	1.768186
7 B	3.601509	1.757083	2.879785	1.765052	1.764778
8 B	2.341814	2.859041	1.800726	2.856932	2.857004
9 C	2.313254	2.729203	2.778137	1.703026	2.732703
10 B	3.621541	2.851941	2.888074	3.355074	1.764575
11 C	2.329385	3.200581	2.771811	2.735790	2.723945
12 B	3.628542	2.845602	3.396991	2.860475	1.758384
13 N	1.827184	4.512521	3.442813	2.893105	5.527058
14 C	1.972451	4.725391	3.004338	3.867268	5.461553
15 C	1.991812	5.363192	4.236904	4.051406	5.536327
	6	7	8	9	10
6 B	0.000000				
7 B	2.846367	0.000000			
8 B	1.761104	3.347060	0.000000		
9 C	3.204011	1.683128	2.729998	0.000000	
10 B	1.765808	2.843840	1.759188	2.723452	0.000000
11 C	2.714630	2.719452	1.678284	1.613825	1.673643
12 B	2.848629	1.754795	2.851492	1.691220	1.757494
13 N	5.034888	4.462233	4.075025	3.362967	5.303792
14 C	4.253228	5.266907	2.876882	4.183755	4.592512
15 C	5.136293	4.930830	3.554184	3.290269	4.540030
	11	12	13	14	15
11 C	0.000000				

	12	B	1.692409	0.000000		
	13	N	3.996095	4.982998	0.000000	
	14	C	3.701628	5.207482	2.773300	0.000000
	15	C	2.960890	4.408532	2.805308	2.829755 0.000000

Table 5C. Energy ranking for (CO)₂(NO)ReC₂B₉H₁₁ obtained after B3LYP/6-31G(d)//SDD optimization:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	03-Anticuboh-Re2-c----259_i-11	-741.4554829	0.00
2	03-Anticuboh-Re3-c----302	-741.4554667	0.01
3	03-Anticuboh-Re3-e----327	-741.4554654	0.01
4	03-Anticuboh-Re3-c----307	-741.4554642	0.01
5	03-Anticuboh-Re3-c----303	-741.4554551	0.02
6	03-Anticuboh-Re3-g----346	-741.4554551	0.02
7	03-Anticuboh-Re2-c----259_r-11	-741.4554386	0.03
8	02-Cuboctaedru-Re2-j----170	-741.4554043	0.05
9	02-Cuboctaedru-Re2-j----168	-741.4553572	0.08
10	02-Cuboctaedru-Re2-f----128	-741.4553485	0.08
11	02-Cuboctaedru-Re1-a----39	-741.4553356	0.09
12	03-Anticuboh-Re2-c----257	-741.4553018	0.11
13	03-Anticuboh-Re3-a----287	-741.4552981	0.12
14	03-Anticuboh-Re3-c----309	-741.4552946	0.12
15	02-Cuboctaedru-Re2-c----96_i-15	-741.4552899	0.12
16	02-Cuboctaedru-Re2-i----155_i-16	-741.4552897	0.12
17	02-Cuboctaedru-Re2-c----96_r-15	-741.4552717	0.13
18	02-Cuboctaedru-Re2-e----112_i-11	-741.4552701	0.13
19	02-Cuboctaedru-Re2-i----155_r-16	-741.4552697	0.13
20	02-Cuboctaedru-Re2-h----142_i-11	-741.4552689	0.13
21	03-Anticuboh-Re2-a----236	-741.4552687	0.13
22	03-Anticuboh-Re3-e----328	-741.4552565	0.14
23	02-Cuboctaedru-Re2-b----87	-741.4552562	0.14
24	02-Cuboctaedru-Re2-j----164	-741.4552553	0.14
25	02-Cuboctaedru-Re2-e----112_r-11	-741.4552334	0.16
26	02-Cuboctaedru-Re2-h----142_r-11	-741.4552325	0.16
27	02-Cuboctaedru-Re1-c----52	-741.4552258	0.16

28	03-Anticuboh-Re3-b----296	-741.4550317	0.28
29	03-Anticuboh-Re3-c----305	-741.4550317	0.28
30	03-Anticuboh-Re3-b----298	-741.4549947	0.31
31	03-Anticuboh-Re3-c----304	-741.4549826	0.31
32	02-Cuboctaedru-Re1-c----57	-741.4549493	0.33
33	02-Cuboctaedru-Re2-f---123	-741.4549234	0.35
34	02-Cuboctaedru-Re2-d----107	-741.4548989	0.37
35	02-Cuboctaedru-Re2-i----160	-741.4548964	0.37
36	02-Cuboctaedru-Re2-h----148_i-31	-741.4546571	0.52
37	02-Cuboctaedru-Re2-h----148_r-31	-741.4546173	0.54
38	02-Cuboctaedru-Re2-f---126	-741.4544943	0.62
39	02-Cuboctaedru-Re2-a----78	-741.4544942	0.62
40	03-Anticuboh-Re3-f---332	-741.4544821	0.63
41	03-Anticuboh-Re3-d----315	-741.4544441	0.65
42	03-Anticuboh-Re3-b----300	-741.4544434	0.65
43	03-Anticuboh-Re2-d----270	-741.4544073	0.67
44	03-Anticuboh-Re3-b----291_r-22	-741.4544024	0.68
45	02-Cuboctaedru-Re2-e----120	-741.4525451	1.84
46	02-Cuboctaedru-Re2-d----102	-741.4525444	1.84
47	02-Cuboctaedru-Re1-a----37	-741.4525303	1.85
48	01-Icos-Re-a----9	-741.4525165	1.86
49	01-Icos-Re-b----15	-741.4525132	1.86
50	03-Anticuboh-Re3-a----289	-741.4525083	1.87
51	02-Cuboctaedru-Re2-c---98	-741.4525036	1.87
52	02-Cuboctaedru-Re2-f---125	-741.4524949	1.88
53	02-Cuboctaedru-Re2-d----106	-741.4524835	1.88
54	03-Anticuboh-Re3-b----292	-741.4524818	1.88
55	02-Cuboctaedru-Re2-a----80	-741.4524806	1.88
56	03-Anticuboh-Re3-b----291_i-22	-741.4522230	2.05
57	02-Cuboctaedru-Re2-j----165	-741.4519723	2.20
58	02-Cuboctaedru-Re2-c---97	-741.4519683	2.21

59	01-Icos-Re-a----4	-741.4519503	2.22
60	03-Anticuboh-Re3-c----301	-741.4519359	2.23
61	02-Cuboctaedru-Re2-j----162	-741.4519220	2.23
62	02-Cuboctaedru-Re2-e----117	-741.4519208	2.24
63	02-Cuboctaedru-Re1-a----40	-741.4518986	2.25
64	02-Cuboctaedru-Re2-i----154	-741.4518821	2.26
65	02-Cuboctaedru-Re2-b----86	-741.4518763	2.26
66	02-Cuboctaedru-Re1-b----49	-741.4518728	2.27
67	03-Anticuboh-Re3-e----321	-741.4518604	2.27
68	03-Anticuboh-Re3-e----324	-741.4518421	2.28
69	03-Anticuboh-Re2-c----251	-741.4518415	2.29
70	02-Cuboctaedru-Re2-b----83	-741.4518333	2.29
71	02-Cuboctaedru-Re2-a----76	-741.4518310	2.29
72	02-Cuboctaedru-Re2-i----156	-741.4518302	2.29
73	03-Anticuboh-Re3-f----338	-741.4518270	2.29
74	03-Anticuboh-Re3-c----310	-741.4518099	2.30
75	03-Anticuboh-Re3-d----317	-741.4518099	2.30
76	03-Anticuboh-Re3-e----325	-741.4518077	2.31
77	03-Anticuboh-Re3-b----297	-741.4518015	2.31
78	03-Anticuboh-Re3-d----312	-741.4517837	2.32
79	03-Anticuboh-Re2-c----260	-741.4517804	2.32
80	02-Cuboctaedru-Re1-b----46	-741.4517723	2.33
81	02-Cuboctaedru-Re1-c----55	-741.4517537	2.34
82	02-Cuboctaedru-Re2-c----99	-741.4500586	3.40
83	02-Cuboctaedru-Re2-k----175	-741.4500580	3.40
84	02-Cuboctaedru-Re2-k----172	-741.4500552	3.41
85	02-Cuboctaedru-Re2-e----119	-741.4500550	3.41
86	03-Anticuboh-Re3-a----284	-741.4500529	3.41
87	03-Anticuboh-Re3-d----313	-741.4500212	3.43
88	01-Icos-Re-a----8	-741.4500201	3.43
89	01-Icos-Re-c----29	-741.4500201	3.43

90	03-Anticuboh-Re3-g----350	-741.4500193	3.43
91	02-Cuboctaedru-Re2-a----79	-741.4500136	3.43
92	02-Cuboctaedru-Re1-d----68	-741.4499838	3.45
93	03-Anticuboh-Re3-a----283	-741.4499816	3.45
94	03-Anticuboh-Re3-g----349	-741.4499816	3.45
95	02-Cuboctaedru-Re2-b----89	-741.4499750	3.46
96	02-Cuboctaedru-Re1-d----63	-741.4499453	3.47
97	02-Cuboctaedru-Re2-k----176	-741.4492506	3.91
98	03-Anticuboh-Re2-e----280	-741.4492189	3.93
99	02-Cuboctaedru-Re1-a----38_i-16	-741.4492045	3.94
100	02-Cuboctaedru-Re1-d----64_i-16	-741.4492035	3.94
101	02-Cuboctaedru-Re1-a----38_r-16	-741.4491835	3.95
102	02-Cuboctaedru-Re1-d----64_r-16	-741.4491835	3.95
103	03-Anticuboh-Re3-e----323	-741.4491634	3.97
104	03-Anticuboh-Re3-g----347	-741.4491634	3.97
105	02-Cuboctaedru-Re1-a----35	-741.4489296	4.11
106	02-Cuboctaedru-Re2-e----115	-741.4489289	4.11
107	03-Anticuboh-Re3-a----281	-741.4489251	4.12
108	02-Cuboctaedru-Re2-a----72	-741.4489247	4.12
109	03-Anticuboh-Re1-a----189	-741.4489076	4.13
110	03-Anticuboh-Re3-d----318	-741.4489000	4.13
111	03-Anticuboh-Re3-e----330	-741.4489000	4.13
112	02-Cuboctaedru-Re1-b----43	-741.4488717	4.15
113	01-Icos-Re-a----5	-741.4488495	4.16
114	02-Cuboctaedru-Re1-b----41	-741.4483345	4.49
115	02-Cuboctaedru-Re2-e----114	-741.4483114	4.50
116	02-Cuboctaedru-Re2-c----92	-741.4483095	4.50
117	03-Anticuboh-Re3-a----286	-741.4482945	4.51
118	03-Anticuboh-Re3-f----339	-741.4482924	4.51
119	01-Icos-Re-a----6	-741.4482679	4.53
120	02-Cuboctaedru-Re1-a----33	-741.4482560	4.54

121	02-Cuboctaedru-Re1-c----56_r-23	-741.4301205	15.92
122	02-Cuboctaedru-Re2-f----130	-741.4300749	15.94
123	02-Cuboctaedru-Re2-d----109	-741.4300688	15.95
124	03-Anticuboh-Re3-f----336	-741.4294066	16.36
125	03-Anticuboh-Re3-c----306	-741.4294041	16.36
126	03-Anticuboh-Re3-b----294	-741.4293865	16.38
127	03-Anticuboh-Re3-f----333	-741.4293772	16.38
128	02-Cuboctaedru-Re2-j----163	-741.4293664	16.39
129	02-Cuboctaedru-Re2-h----147	-741.4293641	16.39
130	03-Anticuboh-Re3-f----335	-741.4293319	16.41
131	03-Anticuboh-Re3-b----295	-741.4293313	16.41
132	02-Cuboctaedru-Re2-h----150	-741.4292235	16.48
133	02-Cuboctaedru-Re2-i----157	-741.4292092	16.49
134	02-Cuboctaedru-Re2-f----127	-741.4292046	16.49
135	02-Cuboctaedru-Re2-i----158	-741.4292045	16.49
136	02-Cuboctaedru-Re2-d----103_r-54	-741.4291329	16.54
137	03-Anticuboh-Re3-g----343	-741.4290666	16.58
138	02-Cuboctaedru-Re1-d----67	-741.4290573	16.58
139	03-Anticuboh-Re2-b----244	-741.4290127	16.61
140	03-Anticuboh-Re2-e----274	-741.4290117	16.61
141	03-Anticuboh-Re2-e----275	-741.4289975	16.62
142	02-Cuboctaedru-Re1-c----58	-741.4289830	16.63
143	02-Cuboctaedru-Re1-d----62	-741.4289827	16.63
144	03-Anticuboh-Re3-b----293	-741.4289823	16.63
145	03-Anticuboh-Re3-g----344	-741.4289823	16.63
146	03-Anticuboh-Re2-c----255	-741.4289747	16.63
147	03-Anticuboh-Re2-e----276	-741.4289438	16.65
148	02-Cuboctaedru-Re2-f----129	-741.4289261	16.66
149	02-Cuboctaedru-Re2-k----179	-741.4289238	16.67
150	02-Cuboctaedru-Re2-i----159	-741.4289225	16.67
151	02-Cuboctaedru-Re2-k----177	-741.4289217	16.67

152	02-Cuboctaedru-Re2-d----110	-741.4289116	16.67
153	02-Cuboctaedru-Re2-k----180	-741.4289108	16.67
154	02-Cuboctaedru-Re1-c----56_i-23	-741.4288921	16.69
155	02-Cuboctaedru-Re2-h----149	-741.4288451	16.72
156	02-Cuboctaedru-Re2-d----103_i-54	-741.4288446	16.72
157	02-Cuboctaedru-Re2-k----173	-741.4288428	16.72
158	03-Anticuboh-Re3-g----345	-741.4288330	16.72
159	02-Cuboctaedru-Re2-j----167	-741.4286901	16.81
160	03-Anticuboh-Re3-f----334	-741.4285298	16.91
161	02-Cuboctaedru-Re1-d----70	-741.4284978	16.93
162	03-Anticuboh-Re3-g----348	-741.4284748	16.95
163	02-Cuboctaedru-Re2-k----178	-741.4284595	16.96
164	02-Cuboctaedru-Re1-d----69	-741.4284257	16.98
165	03-Anticuboh-Re2-a----234	-741.4261271	18.42
166	03-Anticuboh-Re2-b----248	-741.4261271	18.42
167	02-Cuboctaedru-Re2-c----100	-741.4260989	18.44
168	02-Cuboctaedru-Re2-d----105	-741.4260984	18.44
169	01-Icos-Re-b----19	-741.4260702	18.46
170	02-Cuboctaedru-Re2-f----122	-741.4260695	18.46
171	01-Icos-Re-a----2	-741.4260687	18.46
172	02-Cuboctaedru-Re2-e----118	-741.4260684	18.46
173	03-Anticuboh-Re2-b----243	-741.4260599	18.46
174	02-Cuboctaedru-Re2-d----104	-741.4260408	18.48
175	02-Cuboctaedru-Re2-b----90	-741.4260406	18.48
176	02-Cuboctaedru-Re1-b----50	-741.4258849	18.57
177	02-Cuboctaedru-Re1-c----54	-741.4258750	18.58
178	02-Cuboctaedru-Re1-b----42	-741.4258723	18.58
179	02-Cuboctaedru-Re2-i----152_i-14	-741.4255342	18.79
180	02-Cuboctaedru-Re2-e----116_i-14	-741.4255326	18.79
181	03-Anticuboh-Re2-d----262	-741.4255206	18.80
182	02-Cuboctaedru-Re1-c----53	-741.4255062	18.81

183	02-Cuboctaedru-Re1-a----32	-741.4255028	18.81
184	03-Anticuboh-Re3-a----288	-741.4254935	18.82
185	03-Anticuboh-Re3-e----329	-741.4254935	18.82
186	03-Anticuboh-Re3-a----285	-741.4254842	18.82
187	03-Anticuboh-Re3-b----299	-741.4254842	18.82
188	03-Anticuboh-Re3-c----308	-741.4254751	18.83
189	02-Cuboctaedru-Re2-e----116_r-14	-741.4254575	18.84
190	02-Cuboctaedru-Re2-i----152_r-14	-741.4254550	18.84
191	03-Anticuboh-Re2-c----258	-741.4254546	18.84
192	03-Anticuboh-Re2-a----237	-741.4254545	18.84
193	03-Anticuboh-Re3-a----282	-741.4254183	18.87
194	02-Cuboctaedru-Re2-c----94	-741.4243937	19.51
195	02-Cuboctaedru-Re2-b----84	-741.4243810	19.52
196	02-Cuboctaedru-Re2-b----85_i-14	-741.4243785	19.52
197	02-Cuboctaedru-Re2-a----74	-741.4243531	19.53
198	03-Anticuboh-Re2-a----233	-741.4243507	19.54
199	03-Anticuboh-Re2-b----247	-741.4243476	19.54
200	02-Cuboctaedru-Re2-b----85_r-14	-741.4243250	19.55
201	02-Cuboctaedru-Re1-a----31	-741.4243106	19.56
202	02-Cuboctaedru-Re2-b----82	-741.4242836	19.58
203	02-Cuboctaedru-Re2-e----113	-741.4242831	19.58
204	02-Cuboctaedru-Re1-a----34	-741.4236802	19.96
205	02-Cuboctaedru-Re1-b----44	-741.4236802	19.96
206	03-Anticuboh-Re1-b----194	-741.4236073	20.00
207	03-Anticuboh-Re3-f----340	-741.4219124	21.07
208	03-Anticuboh-Re3-d----316	-741.4219118	21.07
209	03-Anticuboh-Re2-a----240	-741.4144438	25.75
210	03-Anticuboh-Re3-a----290	-741.4144348	25.76
211	03-Anticuboh-Re3-d----320	-741.4144328	25.76
212	03-Anticuboh-Re2-b----249	-741.4085586	29.45
213	01-Icos-Re-a----10	-741.4009226	34.24

214	03-Anticuboh-Re1-b----198	-741.4009182	34.24
215	03-Anticuboh-Re1-a----185	-741.4006447	34.41
216	03-Anticuboh-Re1-e----223	-741.3999037	34.88
217	02-Cuboctaedru-Re2-d----101	-741.3994517	35.16
218	02-Cuboctaedru-Re2-g----131	-741.3994517	35.16
219	01-Icos-Re-b----14	-741.3994362	35.17
220	03-Anticuboh-Re2-b----245	-741.3989969	35.45
221	02-Cuboctaedru-Re2-h----146	-741.3989049	35.50
222	02-Cuboctaedru-Re2-i----153	-741.3989049	35.50
223	01-Icos-Re-b----13	-741.3986446	35.67
224	03-Anticuboh-Re2-c----254	-741.3977438	36.23
225	03-Anticuboh-Re2-b----246	-741.3977414	36.23
226	01-Icos-Re-b----20	-741.3975185	36.37
227	03-Anticuboh-Re2-c----253	-741.3975144	36.38
228	03-Anticuboh-Re1-b----193	-741.3966775	36.90
229	03-Anticuboh-Re2-d----265	-741.3965377	36.99
230	03-Anticuboh-Re1-e----225	-741.3963549	37.10
231	03-Anticuboh-Re1-a----184	-741.3963522	37.11
232	03-Anticuboh-Re1-d----215	-741.3963302	37.12
233	03-Anticuboh-Re2-b----241	-741.3963232	37.12
234	03-Anticuboh-Re1-e----226	-741.3956813	37.53
235	03-Anticuboh-Re1-a----190	-741.3956694	37.53
236	03-Anticuboh-Re1-e----222	-741.3956671	37.54
237	03-Anticuboh-Re2-e----273	-741.3955774	37.59
238	01-Icos-Re-c----27	-741.3955723	37.60
239	03-Anticuboh-Re1-c----203	-741.3955346	37.62
240	03-Anticuboh-Re1-c----207	-741.3955165	37.63
241	03-Anticuboh-Re1-c----209	-741.3947292	38.12
242	03-Anticuboh-Re1-e----224	-741.3945614	38.23
243	02-Cuboctaedru-Re2-g----133	-741.3945577	38.23
244	02-Cuboctaedru-Re2-h----141	-741.3945577	38.23

245	03-Anticuboh-Re1-a----183	-741.3945481	38.24
246	03-Anticuboh-Re2-d----261	-741.3945365	38.25
247	02-Cuboctaedru-Re1-d----61	-741.3943373	38.37
248	03-Anticuboh-Re1-c----204	-741.3939233	38.63
249	03-Anticuboh-Re1-a----186	-741.3938988	38.65
250	03-Anticuboh-Re1-c----202	-741.3938988	38.65
251	01-Icos-Re-c----26	-741.3938739	38.66
252	03-Anticuboh-Re1-c----205	-741.3938075	38.70
253	03-Anticuboh-Re1-c----210	-741.3932649	39.04
254	03-Anticuboh-Re1-e----227	-741.3932649	39.04
255	01-Icos-Re-c----21	-741.3932464	39.05
256	01-Icos-Re-c----25	-741.3932255	39.07
257	02-Cuboctaedru-Re2-k----171	-741.3932235	39.07
258	02-Cuboctaedru-Re2-g----140	-741.3932200	39.07
259	03-Anticuboh-Re1-d----214	-741.3923796	39.60
260	03-Anticuboh-Re1-d----213	-741.3922652	39.67
261	03-Anticuboh-Re1-d----218	-741.3922613	39.67
262	02-Cuboctaedru-Re2-f----121	-741.3892495	41.56
263	02-Cuboctaedru-Re2-g----139	-741.3892495	41.56
264	01-Icos-Re-b----11	-741.3892482	41.56
265	03-Anticuboh-Re1-a----181	-741.3887947	41.85
266	03-Anticuboh-Re1-d----212	-741.3887947	41.85
267	02-Cuboctaedru-Re2-c----91	-741.3887874	41.85
268	02-Cuboctaedru-Re2-g----135	-741.3887874	41.85
269	02-Cuboctaedru-Re1-d----66	-741.3877765	42.49
270	03-Anticuboh-Re3-d----314	-741.3877029	42.53
271	03-Anticuboh-Re3-d----319	-741.3872601	42.81
272	03-Anticuboh-Re2-d----268	-741.3871530	42.88
273	03-Anticuboh-Re2-a----232	-741.3871476	42.88
274	03-Anticuboh-Re1-d----217	-741.3871209	42.90
275	03-Anticuboh-Re2-d----267	-741.3871193	42.90

276	03-Anticuboh-Re1-c----201	-741.3871186	42.90
277	02-Cuboctaedru-Re1-a----36	-741.3870975	42.91
278	02-Cuboctaedru-Re2-a----77	-741.3864328	43.33
279	02-Cuboctaedru-Re2-j----166	-741.3864327	43.33
280	03-Anticuboh-Re2-a----239	-741.3864156	43.34
281	03-Anticuboh-Re3-f----331	-741.3863996	43.35
282	03-Anticuboh-Re2-a----235	-741.3863563	43.38
283	03-Anticuboh-Re2-e----278	-741.3863563	43.38
284	03-Anticuboh-Re2-e----277	-741.3863262	43.40
285	03-Anticuboh-Re3-g----341	-741.3863178	43.40
286	02-Cuboctaedru-Re2-b----81	-741.3856764	43.80
287	02-Cuboctaedru-Re2-g----134	-741.3856738	43.81
288	03-Anticuboh-Re2-b----250	-741.3856540	43.82
289	03-Anticuboh-Re2-a----238	-741.3846373	44.46
290	03-Anticuboh-Re1-b----197	-741.3840193	44.84
291	02-Cuboctaedru-Re1-c----51	-741.3819720	46.13
292	02-Cuboctaedru-Re2-h----143	-741.3819601	46.14
293	02-Cuboctaedru-Re2-b----88	-741.3819061	46.17
294	02-Cuboctaedru-Re2-f----124	-741.3819061	46.17
295	02-Cuboctaedru-Re2-k----174	-741.3811138	46.67
296	01-Icos-Re-b----12	-741.3735840	51.39
297	03-Anticuboh-Re1-c----206	-741.3729202	51.81
298	01-Icos-Re-c----24	-741.3729196	51.81
299	01-Icos-Re-c----23	-741.3728923	51.83
300	01-Icos-Re-b----18	-741.3727258	51.93
301	01-Icos-Re-a----1	-741.3722640	52.22
302	01-Icos-Re-c----28	-741.3717126	52.57
303	01-Icos-Re-c----30	-741.3715883	52.65
304	03-Anticuboh-Re2-e----271	-741.3715042	52.70
305	01-Icos-Re-b----17	-741.3713608	52.79
306	01-Icos-Re-c----22	-741.3713608	52.79

307	01-Icos-Re-a----7	-741.3713320	52.81
308	01-Icos-Re-a----3	-741.3711104	52.95
309	01-Icos-Re-b----16	-741.3710884	52.96
310	03-Anticuboh-Re2-b----242	-741.3709156	53.07
311	03-Anticuboh-Re2-d----263	-741.3709156	53.07
312	03-Anticuboh-Re2-d----269	-741.3697710	53.79
313	02-Cuboctaedru-Re2-a----75	-741.3695059	53.95
314	02-Cuboctaedru-Re2-c----95	-741.3695059	53.95
315	02-Cuboctaedru-Re2-c----93_i-12	-741.3692238	54.13
316	02-Cuboctaedru-Re2-h----144_i-12	-741.3692238	54.13
317	02-Cuboctaedru-Re2-c----93_r-12	-741.3691866	54.15
318	02-Cuboctaedru-Re2-h----144_r-12	-741.3691866	54.15
319	02-Cuboctaedru-Re1-d----65	-741.3691292	54.19
320	02-Cuboctaedru-Re1-b----48	-741.3691279	54.19
321	03-Anticuboh-Re1-b----199	-741.3690713	54.23
322	02-Cuboctaedru-Re1-c----59	-741.3681986	54.77
323	03-Anticuboh-Re2-c----256	-741.3681903	54.78
324	03-Anticuboh-Re1-b----191	-741.3679023	54.96
325	03-Anticuboh-Re1-d----219	-741.3679023	54.96
326	02-Cuboctaedru-Re2-a----73	-741.3678916	54.97
327	02-Cuboctaedru-Re2-h----145	-741.3678916	54.97
328	03-Anticuboh-Re3-e----326	-741.3657342	56.32
329	03-Anticuboh-Re3-f----337	-741.3657259	56.32
330	03-Anticuboh-Re1-d----216	-741.3654017	56.53
331	02-Cuboctaedru-Re2-g----137	-741.3653635	56.55
332	02-Cuboctaedru-Re2-i----151	-741.3653635	56.55
333	02-Cuboctaedru-Re2-g----138	-741.3647376	56.94
334	02-Cuboctaedru-Re2-j----161	-741.3647376	56.94
335	03-Anticuboh-Re1-b----196	-741.3640724	57.36
336	03-Anticuboh-Re1-d----211	-741.3623125	58.47
337	03-Anticuboh-Re1-e----221	-741.3623125	58.47

338	02-Cuboctaedru-Re2-a----71	-741.3622751	58.49
339	02-Cuboctaedru-Re2-g----136	-741.3622751	58.49
340	03-Anticuboh-Re1-d----220	-741.3622660	58.50
341	02-Cuboctaedru-Re1-b----47	-741.3597058	60.10
342	03-Anticuboh-Re3-d----311	-741.3554948	62.74
343	02-Cuboctaedru-Re2-e----111	-741.3551186	62.98
344	02-Cuboctaedru-Re2-g----132	-741.3551186	62.98
345	03-Anticuboh-Re2-c----252	-741.3486355	67.05
346	03-Anticuboh-Re2-d----266	-741.3486355	67.05
347	03-Anticuboh-Re2-e----279	-741.3406244	72.08
348	02-Cuboctaedru-Re2-j----169	-741.3405988	72.09
349	03-Anticuboh-Re1-e----230	-741.3400350	72.45
350	03-Anticuboh-Re1-a----182	-741.3363931	74.73
351	03-Anticuboh-Re1-b----200	-741.3362751	74.81
352	03-Anticuboh-Re1-e----229	-741.3362751	74.81
353	03-Anticuboh-Re3-e----322	-741.3332387	76.71
354	03-Anticuboh-Re3-g----342	-741.3290708	79.33
355	03-Anticuboh-Re1-b----192	-741.3283004	79.81
356	03-Anticuboh-Re1-a----188	-741.3282948	79.81
357	02-Cuboctaedru-Re1-c----60	-741.3257130	81.43
358	03-Anticuboh-Re1-e----228	-741.3237747	82.65
359	02-Cuboctaedru-Re1-b----45	-741.3115816	90.30
360	02-Cuboctaedru-Re2-d----108	-741.2952580	100.54
361	03-Anticuboh-Re2-a----231_i-51	-741.2952028	100.58
362	03-Anticuboh-Re2-a----231_r-51	-741.2951297	100.62
363	03-Anticuboh-Re1-c----208	-741.2948456	100.80
364	03-Anticuboh-Re1-b----195	-741.2933919	101.72
365	03-Anticuboh-Re2-d----264	-741.2884455	104.82
366	03-Anticuboh-Re2-e----272	-741.2884455	104.82
367	03-Anticuboh-Re1-a----187	-741.2737998	114.01

Table 6S. Orbital energies and HOMO-LUMO gaps of the lowest lying structures.

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	Gap (Hartree)	Gap (eV)
01-08v-ReC2H2BnHn	-0.236287	-0.128431	0.107856	2.93
02-08v-ReC2H2BnHn	-0.237304	-0.128033	0.109271	2.97
03-08v-ReC2H2BnHn	-0.235699	-0.136986	0.098713	2.69
04-08v-ReC2H2BnHn	-0.232647	-0.137983	0.094664	2.58
05-08v-ReC2H2BnHn	-0.222361	-0.130688	0.091673	2.49
06-08v-ReC2H2BnHn	-0.228813	-0.137349	0.091464	2.49
01-09v-ReC2H2BnHn	-0.227717	-0.135226	0.092491	2.52
02-09v-ReC2H2BnHn	-0.238346	-0.133710	0.104636	2.85
03-09v-ReC2H2BnHn	-0.224069	-0.131786	0.092283	2.51
04-09v-ReC2H2BnHn	-0.228472	-0.139580	0.088892	2.42
05-09v-ReC2H2BnHn	-0.221451	-0.139136	0.082315	2.24
06-09v-ReC2H2BnHn	-0.216942	-0.133682	0.083260	2.27
07-09v-ReC2H2BnHn	-0.222651	-0.138458	0.084193	2.29
08-09v-ReC2H2BnHn	-0.221953	-0.136392	0.085561	2.33
09-09v-ReC2H2BnHn	-0.236834	-0.138228	0.098606	2.68
01-10v-ReC2H2BnHn	-0.241560	-0.132646	0.108914	2.96
02-10v-ReC2H2BnHn	-0.247164	-0.136235	0.110929	3.02
03-10v-ReC2H2BnHn	-0.239196	-0.129222	0.109974	2.99
04-10v-ReC2H2BnHn	-0.240348	-0.134791	0.105557	2.87
05-10v-ReC2H2BnHn	-0.240311	-0.130533	0.109778	2.99
06-10v-ReC2H2BnHn	-0.231321	-0.126172	0.105149	2.86
07-10v-ReC2H2BnHn	-0.240301	-0.139946	0.100355	2.73
01-11v-ReC2H2BnHn	-0.238562	-0.150160	0.088402	2.41
02-11v-ReC2H2BnHn	-0.220297	-0.138191	0.082106	2.23
03-11v-ReC2H2BnHn	-0.237305	-0.132087	0.105218	2.86
04-11v-ReC2H2BnHn	-0.226523	-0.147881	0.078642	2.14
05-11v-ReC2H2BnHn	-0.230574	-0.135536	0.095038	2.59
06-11v-ReC2H2BnHn	-0.243503	-0.136742	0.106761	2.91
07-11v-ReC2H2BnHn	-0.234233	-0.134471	0.099762	2.71
08-11v-ReC2H2BnHn	-0.241938	-0.137429	0.104509	2.84
09-11v-ReC2H2BnHn	-0.235438	-0.138952	0.096486	2.63
10-11v-ReC2H2BnHn	-0.233097	-0.140840	0.092257	2.51
01-12v-ReC2H2BnHn	-0.238068	-0.128287	0.109781	2.99
02-12v-ReC2H2BnHn	-0.241725	-0.137008	0.104717	2.85
03-12v-ReC2H2BnHn	-0.246246	-0.138350	0.107896	2.94
04-12v-ReC2H2BnHn	-0.238702	-0.134978	0.103724	2.82
05-12v-ReC2H2BnHn	-0.252472	-0.148645	0.103827	2.83
06-12v-ReC2H2BnHn	-0.236556	-0.126736	0.109820	2.99
07-12v-ReC2H2BnHn	-0.234142	-0.124456	0.109686	2.98
08-12v-ReC2H2BnHn	-0.244257	-0.137933	0.106324	2.89

09-12v-ReC2H2BnHn	-0.251985	-0.151910	0.100075	2.72
10-12v-ReC2H2BnHn	-0.251138	-0.146337	0.104801	2.85