Supporting Information

Manganese-centered Ten-vertex Germanium Clusters: The Strong Field Ge_{10} Ligand Encapsulating a Transition Metal

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- Tables of distances for the $Mn@Ge_{10}^{z}$ derivatives (z = –5 to +1).

- Tables of distances for the $Mn@Ge_{10}^{z}$ derivatives in THF (z = –2 to +1).

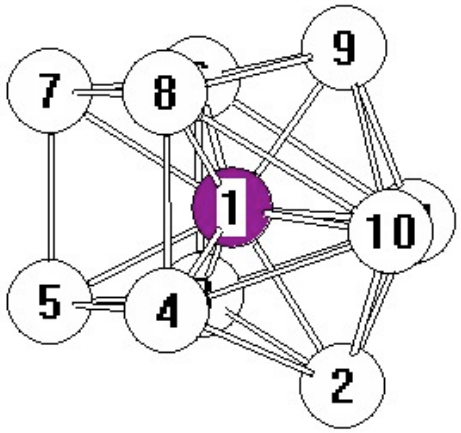
- Complete Gaussian reference (reference 30).

$Mn@Ge_{10}^{5-}$

Charge 5-

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.594596	0.000000				
3 Ge	2.388375	2.987603	0.000000			
4 Ge	2.388375	2.987603	3.975478	0.000000		
5 Ge	2.557103	3.773336	2.586439	2.586439	0.000000	
6 Ge	2.483197	4.618357	2.692709	4.695146	3.660034	
7 Ge	2.683186	5.144423	3.675803	3.675803	2.622444	
8 Ge	2.483197	4.618357	4.695146	2.692709	3.660034	
9 Ge	2.434431	4.203652	4.245548	4.245548	4.847982	
10 Ge	2.516908	2.528511	4.425029	2.932583	4.674155	
11 Ge	2.516908	2.528511	2.932583	4.425029	4.674155	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.472107	0.000000				
8 Ge	3.721240	2.472107	0.000000			
9 Ge	2.796061	3.699002	2.796061	0.000000		
10 Ge	4.579580	4.862002	3.270161	2.702317	0.000000	
11 Ge	3.270161	4.862002	4.579580	2.702317	2.762143	0.000000



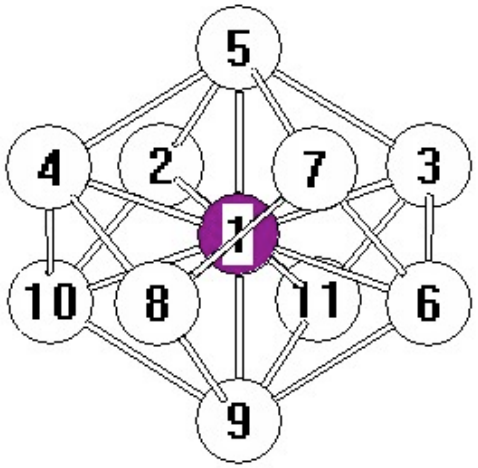
0-3 CCD – C_s [1] [9]

- 21900.4220019 (+27.07 kcal/mol) ** i -32 **

Charge 5-

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.598694	0.000000				
3 Ge	2.597573	3.491348	0.000000			
4 Ge	2.597573	3.491348	4.938480	0.000000		
5 Ge	2.238756	2.857437	2.854626	2.854626	0.000000	
6 Ge	2.597409	4.839085	2.482761	4.840565	3.917897	
7 Ge	2.592665	4.934485	3.489893	3.489893	2.848337	
8 Ge	2.597409	4.839085	4.840565	2.482761	3.917897	
9 Ge	2.238601	3.922496	3.920334	3.920334	4.477355	
10 Ge	2.595662	2.483205	4.836308	2.482678	3.919743	
11 Ge	2.595662	2.483205	2.482678	4.836308	3.919743	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.483146	0.000000				
8 Ge	3.496413	2.483146	0.000000			
9 Ge	2.855110	3.915684	2.855110	0.000000		
10 Ge	4.937378	4.833268	3.490225	2.854692	0.000000	
11 Ge	3.490225	4.833268	4.937378	2.854692	3.488155	0.000000



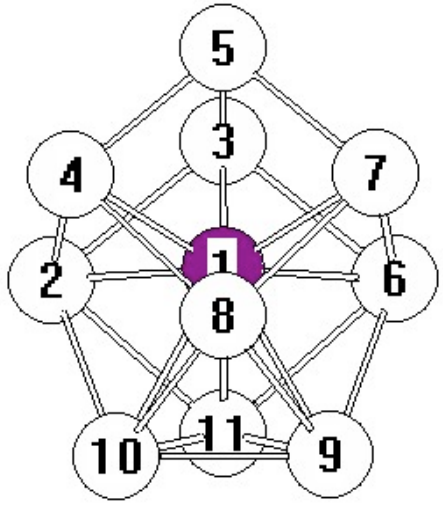
0-3 CCD – C_s [1] (r-32) → C_s [1] [4]

- 21900.4374111 (+17.40 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.432569	0.000000				
3	Ge	2.485350	2.771683	0.000000			
4	Ge	2.485350	2.771683	3.685294	0.000000		
5	Ge	2.672616	3.818123	2.540688	2.540688	0.000000	
6	Ge	2.432525	4.184233	2.771460	4.806680	3.817934	
7	Ge	2.485291	4.806703	3.685513	3.685513	2.540610	
8	Ge	2.432525	4.184233	4.806680	2.771460	3.817934	
9	Ge	2.654116	4.356433	4.694516	4.694516	5.087472	
10	Ge	2.654041	2.844896	4.694538	3.528791	5.087709	
11	Ge	2.654041	2.844896	3.528791	4.694538	5.087709	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.772048	0.000000				
8	Ge	4.185062	2.772048	0.000000			
9	Ge	2.844606	3.528120	2.844606	0.000000		
10	Ge	4.355939	4.694095	2.843918	2.601133	0.000000	
11	Ge	2.843918	4.694095	4.355939	2.601133	2.601236	0.000000



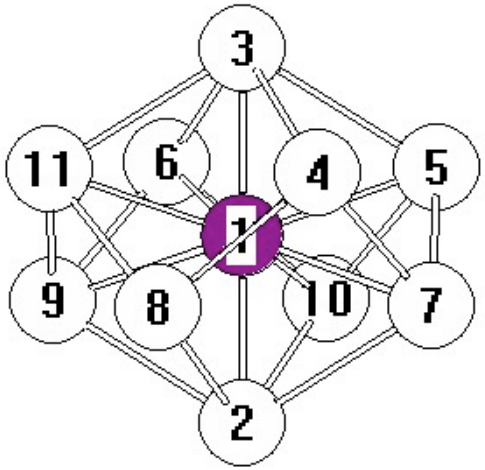
0-3 CCD – C_s [3] **[7]**

- 21900.4299204 (+22.10 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.239235	0.000000				
3	Ge	2.239201	4.478436	0.000000			
4	Ge	2.596838	3.919737	2.855004	0.000000		
5	Ge	2.596838	3.919737	2.855004	3.491427	0.000000	
6	Ge	2.596838	3.919737	2.855004	4.937623	3.491427	
7	Ge	2.596615	2.854438	3.919839	2.482763	2.483334	
8	Ge	2.596615	2.854438	3.919839	2.483334	4.837722	
9	Ge	2.596615	2.854438	3.919839	4.837722	4.837429	
10	Ge	2.596615	2.854438	3.919839	4.837429	2.482763	
11	Ge	2.596838	3.919737	2.855004	3.491427	4.937623	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.837722	0.000000				
8	Ge	4.837429	3.490871	0.000000			
9	Ge	2.482763	4.936837	3.490871	0.000000		
10	Ge	2.483334	3.490871	4.936837	3.490871	0.000000	
11	Ge	3.491427	4.837429	2.482763	2.483334	4.837722	0.000000



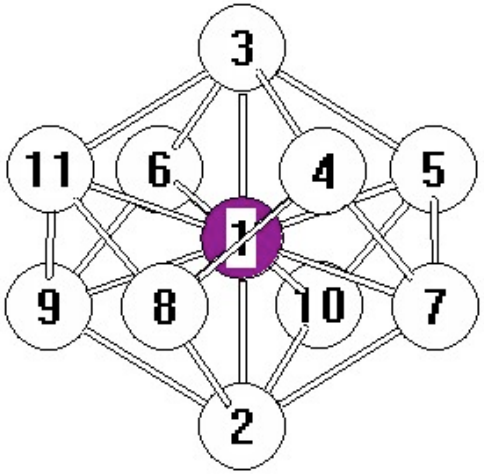
0-4 APT – D_{4d} [1] **(ra-758) → C_4** [1] **[4]**

- 21900.4374010 (+17.41 kcal/mol)

Charge 5-

		1	2	3	4	5	6
1	Mn	0.000000					
2	Ge	2.239313	0.000000				
3	Ge	2.238435	4.477706	0.000000			
4	Ge	2.594113	3.910680	2.847709	0.000000		
5	Ge	2.598428	3.917310	2.852444	3.494076	0.000000	
6	Ge	2.597097	3.925201	2.862137	4.936206	3.494557	0.000000
7	Ge	2.594651	2.842913	3.913239	2.482730	2.484228	4.837191
8	Ge	2.598398	2.850776	3.921235	2.483961	4.842558	4.837108
9	Ge	2.597723	2.862307	3.926816	4.834988	4.839825	2.482282
10	Ge	2.593224	2.852690	3.919139	4.833098	2.482620	2.484228
11	Ge	2.596864	3.921959	2.860177	3.489100	4.940113	3.489496

		7	8	9	10	11
7	Ge	0.000000				
8	Ge	3.492137	0.000000			
9	Ge	4.934709	3.488809	0.000000		
10	Ge	3.486678	4.933456	3.488070	0.000000	
11	Ge	4.836032	2.482556	2.482939	4.833983	0.000000



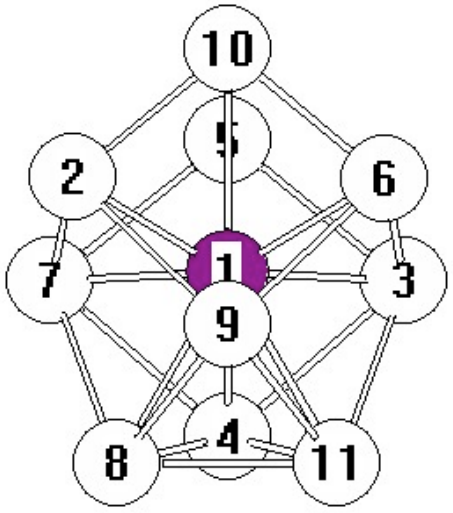
0-4 APT – D_{4d} [1] (rd-65) → C_1 [1] [4]

- 21900.4373589 (+17.44 kcal/mol)

Charge 5-

		1	2	3	4	5	6
1	Mn	0.000000					
2	Ge	2.486272	0.000000				
3	Ge	2.432966	4.806968	0.000000			
4	Ge	2.653982	4.697439	2.843199	0.000000		
5	Ge	2.486113	3.686466	2.769889	3.527536	0.000000	
6	Ge	2.486113	3.686466	2.769889	4.693163	3.685057	0.000000
7	Ge	2.431479	2.770917	4.184438	2.848345	2.770940	4.805715
8	Ge	2.651939	3.531589	4.354523	2.601260	4.693464	4.693464
9	Ge	2.431479	2.770917	4.184438	4.357945	4.805715	2.770940
10	Ge	2.672329	2.540317	3.815101	5.086387	2.540114	5.086387
11	Ge	2.653982	4.697439	2.843199	2.600303	4.693163	3.527536

		7	8	9	10	11
7	Ge	0.000000				
8	Ge	4.805715	0.000000			
9	Ge	4.693464	2.846078	0.000000		
10	Ge	2.770940	4.183597	2.846078	0.000000	
11	Ge	2.540114	3.815286	5.086767	3.815286	0.000000



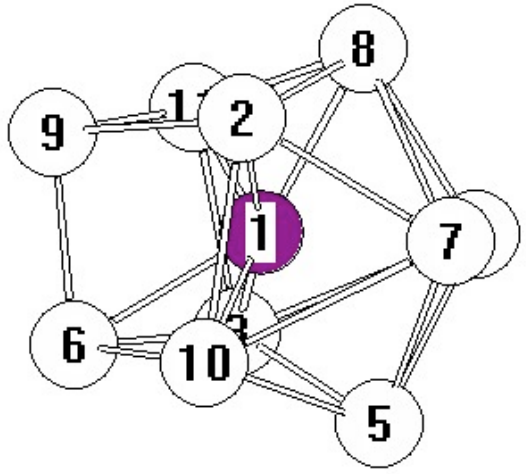
0-4 APT – C_{2v} [3] (ra-70) → C_s [3] [7]

- 21900.4299198 (+22.10 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.345601	0.000000				
3	Ge	2.425888	4.738619	0.000000			
4	Ge	2.675395	4.176320	3.243032	0.000000		
5	Ge	2.675395	4.176320	3.243032	2.847363	0.000000	
6	Ge	2.569542	3.941299	2.665868	4.923077	3.760211	
7	Ge	2.733420	2.841182	4.597694	2.557445	2.557445	
8	Ge	2.479357	2.876417	3.979410	2.575105	4.470437	
9	Ge	2.703237	3.011426	3.746699	5.151751	5.151751	
10	Ge	2.479357	2.876417	3.979410	4.470437	2.575105	
11	Ge	2.569542	3.941299	2.665868	3.760211	4.923077	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.923434	0.000000				
8	Ge	4.832685	3.207422	0.000000			
9	Ge	2.498415	5.114829	3.765164	0.000000		
10	Ge	2.592969	3.207422	4.689829	3.765164	0.000000	
11	Ge	3.546261	4.923434	2.592969	2.498415	4.832685	0.000000



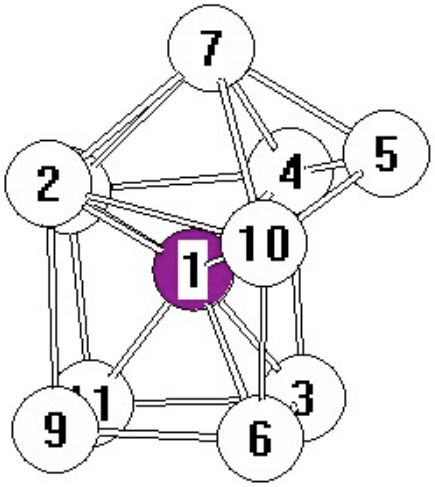
0-4 APT – C_{2v} [3] (rc-45) → C_s [3] [8]

- 21900.4290674 (+22.64 kcal/mol) ** i -42 **

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.354261	0.000000				
3	Ge	2.461297	4.766376	0.000000			
4	Ge	2.548274	4.279634	2.798551	0.000000		
5	Ge	2.786110	4.155761	3.672493	2.757947	0.000000	
6	Ge	2.534177	4.009992	2.707408	4.541955	3.830790	
7	Ge	2.690426	2.761533	4.638505	2.751885	2.502446	
8	Ge	2.463966	2.889867	3.813502	2.714064	4.489325	
9	Ge	2.680522	2.998219	3.716958	5.025319	5.225970	
10	Ge	2.497836	2.928719	4.167403	4.348541	2.542800	
11	Ge	2.623238	3.913639	2.592137	3.722022	5.185219	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.879410	0.000000				
8	Ge	4.808447	3.074636	0.000000			
9	Ge	2.533439	5.026849	3.819804	0.000000		
10	Ge	2.603582	3.247211	4.705053	3.721437	0.000000	
11	Ge	3.571643	4.896097	2.602720	2.485648	4.889689	0.000000



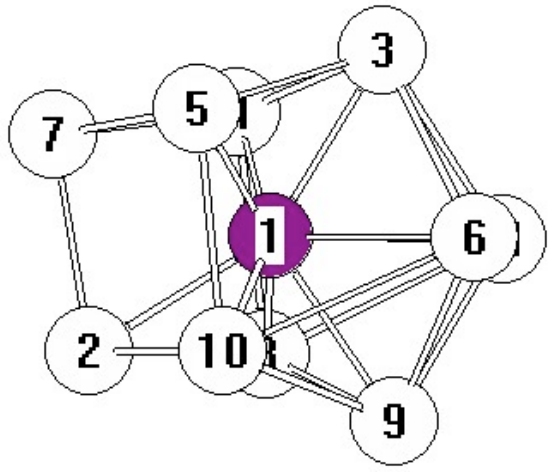
0-4 APT – C_{2v} [3] (rc-45, r-42) → C_1 [3] [6]

- 21900.4305403 (+21.71 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.510327	0.000000				
3	Ge	2.528011	4.902752	0.000000			
4	Ge	2.431348	3.668917	2.756185	0.000000		
5	Ge	2.431348	3.668917	2.756185	3.662311	0.000000	
6	Ge	2.842868	5.026142	2.793755	4.662507	3.577950	
7	Ge	2.815626	2.561537	3.982113	2.668977	2.668977	
8	Ge	2.429312	2.704058	4.351349	2.848545	4.766722	
9	Ge	2.600443	3.682626	4.312445	4.564666	4.564666	
10	Ge	2.429312	2.704058	4.351349	4.766722	2.848545	
11	Ge	2.842868	5.026142	2.793755	3.577950	4.662507	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	5.398726	0.000000				
8	Ge	4.511194	3.940196	0.000000			
9	Ge	2.693341	5.223609	2.779345	0.000000		
10	Ge	3.258438	3.940196	3.988583	2.779345	0.000000	
11	Ge	2.440330	5.398726	3.258438	2.693341	4.511194	0.000000



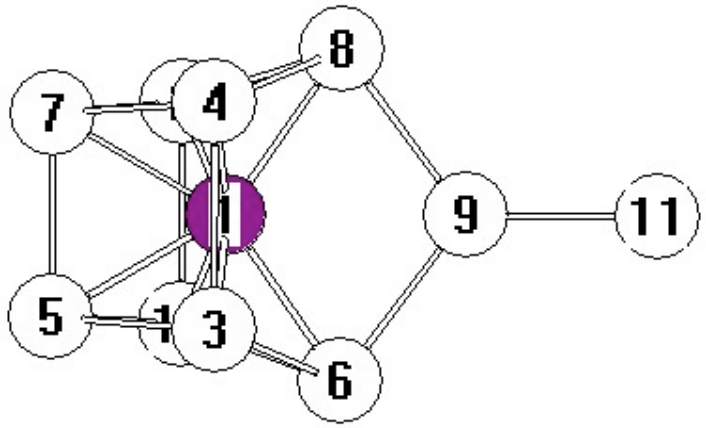
0-4 APT – C_{2v} [5] (rb-237) → C_s [5] [10]

- 21900.4149555 (+31.49 kcal/mol) ** i -38 **

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.405435	0.000000				
3	Ge	2.386517	4.739394	0.000000			
4	Ge	2.387647	3.845908	2.798653	0.000000		
5	Ge	2.506707	3.725325	2.652683	3.751116	0.000000	
6	Ge	2.508789	4.273568	2.778291	4.382425	3.696714	
7	Ge	2.508179	2.645885	3.750274	2.650407	2.514434	
8	Ge	2.508896	2.653619	4.378038	2.774856	4.896768	
9	Ge	3.014064	3.986393	4.239446	4.242072	5.325781	
10	Ge	2.404790	2.733471	3.851722	4.739721	2.647435	
11	Ge	5.335507	6.360626	5.957892	5.962830	7.599313	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.897880	0.000000				
8	Ge	4.100933	3.698490	0.000000			
9	Ge	2.580604	5.328075	2.582854	0.000000		
10	Ge	2.654325	3.725297	4.271219	3.983643	0.000000	
11	Ge	4.428831	7.602721	4.433446	2.471978	6.356973	0.000000



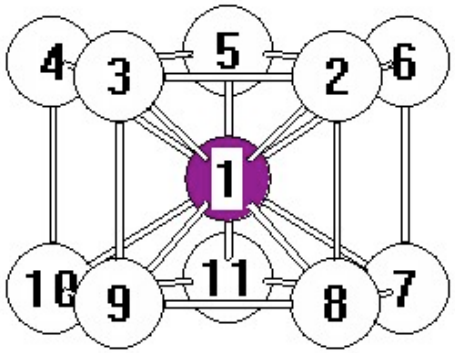
0-4 APT – C_{2v} [5] (rb-237, r-38) → C_1 [5] [3]

- 21900.4458816 (+12.09 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.535907	0.000000				
3	Ge	2.536116	2.542729	0.000000			
4	Ge	2.535356	4.112992	2.541424	0.000000		
5	Ge	2.535367	4.113669	4.113338	2.541973	0.000000	
6	Ge	2.535933	2.542314	4.114098	4.113750	2.543189	
7	Ge	2.535367	3.670314	4.891928	4.892047	3.671729	
8	Ge	2.535356	2.647891	3.670083	4.890828	4.892047	
9	Ge	2.536116	3.670929	2.647564	3.670083	4.891928	
10	Ge	2.535907	4.892429	3.670929	2.647891	3.670314	
11	Ge	2.535933	4.892657	4.892614	3.671347	2.648336	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.648336	0.000000				
8	Ge	3.671347	2.541973	0.000000			
9	Ge	4.892614	4.113338	2.541424	0.000000		
10	Ge	4.892657	4.113669	4.112992	2.542729	0.000000	
11	Ge	3.671702	2.543189	4.113750	4.114098	2.542314	0.000000



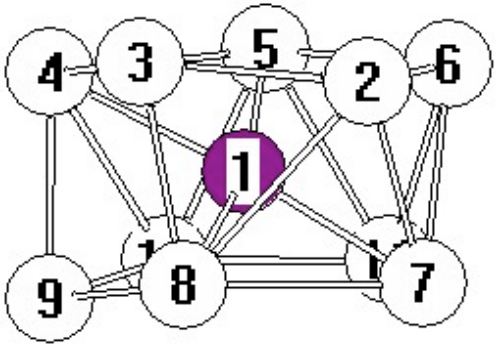
0-5 APP – D_{5d} [1] (rb-99) → C_2 [1] [1]

- 21900.4651447 (**+0.00 kcal/mol**)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.688407	0.000000				
3	Ge	2.704513	2.640502	0.000000			
4	Ge	2.566909	4.415171	2.683196	0.000000		
5	Ge	2.584675	4.350315	4.437489	3.042908	0.000000	
6	Ge	2.694783	2.627683	4.336106	4.608127	2.732478	
7	Ge	2.584676	2.708354	4.340400	5.127387	4.444906	
8	Ge	2.566909	3.186214	2.640380	3.834058	5.127387	
9	Ge	2.704514	4.946311	3.647753	2.640380	4.340400	
10	Ge	2.688408	5.344403	4.946310	3.186214	2.708354	
11	Ge	2.694783	4.398543	5.368978	4.718048	2.865345	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.865345	0.000000				
8	Ge	4.718048	3.042909	0.000000			
9	Ge	5.368978	4.437489	2.683197	0.000000		
10	Ge	4.398543	4.350315	4.415171	2.640502	0.000000	
11	Ge	2.765701	2.732478	4.608127	4.336107	2.627684	0.000000



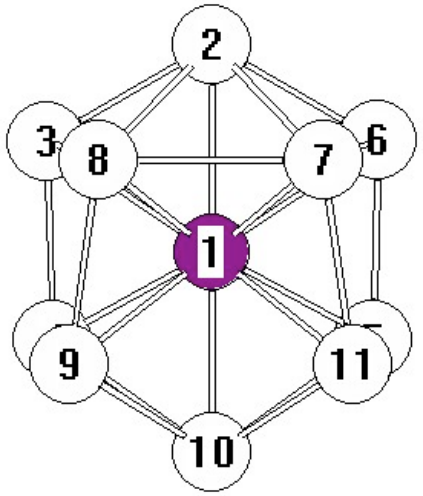
0-5 APP – C_i [7] (ra-38) → C_1 [7] [12]

- 21900.3878224 (+48.52 kcal/mol) ** i -1 **

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.708594	0.000000				
3	Ge	2.728169	2.583003	0.000000			
4	Ge	2.693781	4.511016	2.628418	0.000000		
5	Ge	2.693776	4.511024	4.998961	4.182807	0.000000	
6	Ge	2.728163	2.583008	4.322692	4.998954	2.628422	
7	Ge	2.618453	2.885809	4.488882	5.247212	3.903312	
8	Ge	2.618457	2.885793	2.727905	3.903329	5.247209	
9	Ge	2.699918	4.790744	3.622415	2.605282	4.718822	
10	Ge	2.626862	5.313300	4.623962	2.721239	2.721254	
11	Ge	2.699915	4.790754	5.396242	4.718821	2.605278	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.727902	0.000000				
8	Ge	4.488872	2.939964	0.000000			
9	Ge	5.396241	4.279038	2.725786	0.000000		
10	Ge	4.623973	4.597685	4.597685	2.723616	0.000000	
11	Ge	3.622429	2.725779	4.279035	3.700815	2.723626	0.000000



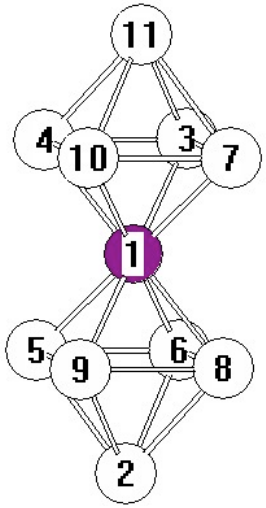
0-5 APP – C_i [7] (rb-22) → C_1 [7] [13]

- 21900.3851920 (+50.17 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.796936	0.000000				
3	Ge	2.566143	5.902396	0.000000			
4	Ge	2.566143	5.902396	2.555462	0.000000		
5	Ge	2.566143	2.676815	4.450839	3.644115	0.000000	
6	Ge	2.566143	2.676815	3.644115	4.450839	2.555462	
7	Ge	2.566143	5.902396	2.555462	3.613970	5.132285	
8	Ge	2.566143	2.676815	4.450839	5.132285	3.613970	
9	Ge	2.566143	2.676815	5.132285	4.450839	2.555462	
10	Ge	2.566143	5.902396	3.613970	2.555462	4.450839	
11	Ge	3.796936	7.593872	2.676815	2.676815	5.902396	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.450839	0.000000				
8	Ge	2.555462	3.644115	0.000000			
9	Ge	3.613970	4.450839	2.555462	0.000000		
10	Ge	5.132285	2.555462	4.450839	3.644115	0.000000	
11	Ge	5.902396	2.676815	5.902396	5.902396	2.676815	0.000000



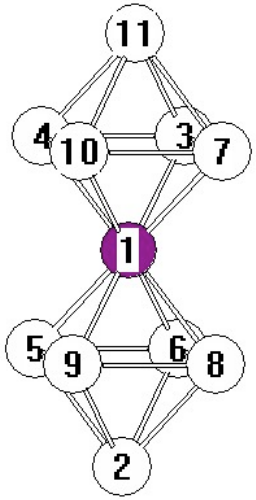
0-8 CBO – D_{4h} [1] [11]

- 21900.4048412 (+37.84 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.817120	0.000000				
3	Ge	2.618574	5.978630	0.000000			
4	Ge	2.618574	5.978630	2.584603	0.000000		
5	Ge	2.618574	2.666581	4.554948	3.750650	0.000000	
6	Ge	2.618574	2.666581	3.750650	4.554948	2.584603	
7	Ge	2.618574	5.978630	2.584603	3.655181	5.237148	
8	Ge	2.618574	2.666581	4.554948	5.237148	3.655181	
9	Ge	2.618574	2.666581	5.237148	4.554948	2.584603	
10	Ge	2.618574	5.978630	3.655181	2.584603	4.554948	
11	Ge	3.817120	7.634240	2.666581	2.666581	5.978630	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.554948	0.000000				
8	Ge	2.584603	3.750650	0.000000			
9	Ge	3.655181	4.554948	2.584603	0.000000		
10	Ge	5.237148	2.584603	4.554948	3.750650	0.000000	
11	Ge	5.978630	2.666581	5.978630	5.978630	2.666581	0.000000



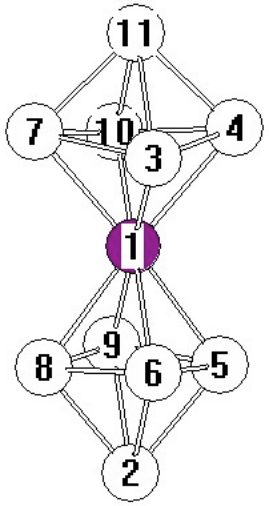
0-8 CBO – D_{4h} [3] [2]

- 21900.4605437 (+2.89 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	4.197143	0.000000				
3	Ge	2.575527	6.316220	0.000000			
4	Ge	2.844475	6.610726	2.594915	0.000000		
5	Ge	2.771934	2.568401	4.756287	4.377299	0.000000	
6	Ge	2.822643	2.852539	3.944384	4.996901	2.527751	
7	Ge	2.844475	6.610726	2.594915	3.739345	5.611908	
8	Ge	2.771934	2.568401	4.756287	5.611908	3.298110	
9	Ge	2.822643	2.852539	5.397938	4.996901	2.527751	
10	Ge	2.575527	6.316220	3.555039	2.594915	4.756287	
11	Ge	3.932490	8.129633	2.727461	2.587570	6.377438	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.996901	0.000000				
8	Ge	2.527751	4.377299	0.000000			
9	Ge	3.819809	4.996901	2.527751	0.000000		
10	Ge	5.397938	2.594915	4.756287	3.944384	0.000000	
11	Ge	6.306983	2.587570	6.377438	6.306983	2.727461	0.000000



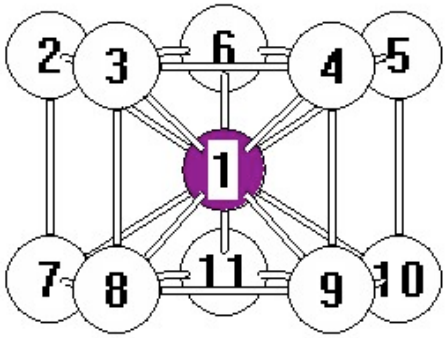
0-8 CBO – D_{2h} [5] (ra-1456) → C_{2v} [5] [5]

- 21900.4364834 (+17.98 kcal/mol)

Charge 5-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.537369	0.000000				
3	Ge	2.537369	2.543705	0.000000			
4	Ge	2.537369	4.115801	2.543705	0.000000		
5	Ge	2.537369	4.115801	4.115801	2.543705	0.000000	
6	Ge	2.537369	2.543705	4.115801	4.115801	2.543705	
7	Ge	2.537369	2.650428	3.673582	4.895364	4.895364	
8	Ge	2.537369	3.673582	2.650428	3.673582	4.895364	
9	Ge	2.537369	4.895364	3.673582	2.650428	3.673582	
10	Ge	2.537369	4.895364	4.895364	3.673582	2.650428	
11	Ge	2.537369	3.673582	4.895364	4.895364	3.673582	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.673582	0.000000				
8	Ge	4.895364	2.543705	0.000000			
9	Ge	4.895364	4.115801	2.543705	0.000000		
10	Ge	3.673582	4.115801	4.115801	2.543705	0.000000	
11	Ge	2.650428	2.543705	4.115801	4.115801	2.543705	0.000000



0-9 PPG – D_{5h} [1] [1]

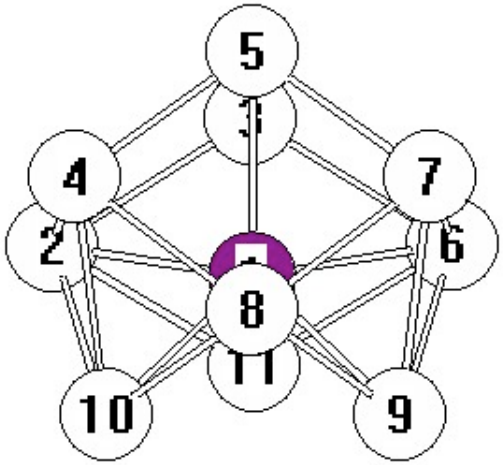
- 21900.4651151 (**+0.02 kcal/mol**)

$Mn@Ge_{10}^{4-}$

Charge 4-

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.578565	0.000000				
3 Ge	2.653314	2.740058	0.000000			
4 Ge	2.653303	2.743580	3.957017	0.000000		
5 Ge	2.546734	3.550937	2.580842	2.580126	0.000000	
6 Ge	2.585906	4.464670	2.739772	5.023481	3.550923	
7 Ge	2.649955	5.016482	3.958990	3.956925	2.581986	
8 Ge	2.589611	4.470002	5.027177	2.741369	3.553265	
9 Ge	2.348542	4.714140	4.543927	4.539850	4.365485	
10 Ge	2.350138	2.762245	4.547743	2.760699	4.366136	
11 Ge	2.349665	2.760984	2.765625	4.547900	4.368811	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.746040	0.000000				
8 Ge	4.483986	2.745279	0.000000			
9 Ge	2.765902	2.755909	2.760775	0.000000		
10 Ge	4.725176	4.532948	2.747399	3.277986	0.000000	
11 Ge	2.747251	4.534487	4.726383	3.279297	3.297338	0.000000



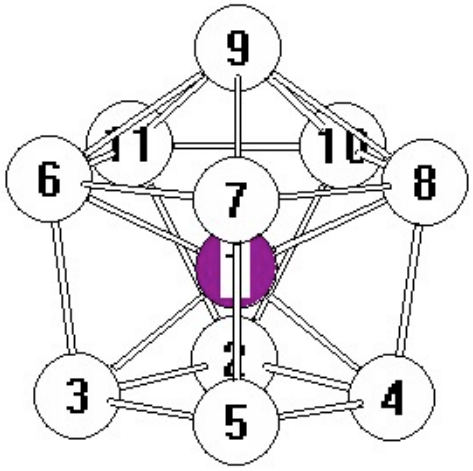
0-3 CCD – C_1 [4] **[10]**

- 21900.8491962 (+57.95 kcal/mol)

Charge 4-

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.448379	0.000000				
3 Ge	2.428223	2.808394	0.000000			
4 Ge	2.428223	2.808394	3.749643	0.000000		
5 Ge	2.519707	3.989359	2.669265	2.669265	0.000000	
6 Ge	2.534861	4.142591	2.701830	4.909087	3.830030	
7 Ge	2.459554	4.898550	3.891360	3.891360	2.715543	
8 Ge	2.534861	4.142591	4.909087	2.701830	3.830030	
9 Ge	2.634245	4.412571	4.578496	4.578496	4.721766	
10 Ge	2.710922	2.857928	4.680434	3.517818	5.060040	
11 Ge	2.710922	2.857928	3.517818	4.680434	5.060040	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.857407	0.000000				
8 Ge	4.480228	2.857407	0.000000			
9 Ge	2.768750	2.801833	2.768750	0.000000		
10 Ge	4.309244	4.456715	2.679749	2.711429	0.000000	
11 Ge	2.679749	4.456715	4.309244	2.711429	2.541954	0.000000



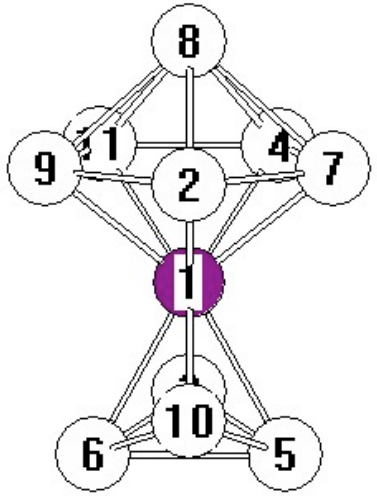
0-3 CCD – C_s [6] **[11]**

- 21900.8491395 (+57.99 kcal/mol) ** i -16 **

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.739348	0.000000				
3	Ge	2.637591	5.369954	0.000000			
4	Ge	2.731813	4.068774	3.767184	0.000000		
5	Ge	2.792079	4.822508	2.465477	4.521282	0.000000	
6	Ge	2.792079	4.822508	2.465477	5.222141	2.716442	
7	Ge	2.728635	2.509602	4.815279	2.504649	4.238717	
8	Ge	3.428580	2.762956	5.594060	2.734544	6.022563	
9	Ge	2.728635	2.509602	4.815279	4.055154	5.381203	
10	Ge	2.620934	3.383509	3.905144	5.196135	2.481353	
11	Ge	2.731813	4.068774	3.767184	2.513865	5.222141	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	5.381203	0.000000				
8	Ge	6.022563	2.739688	0.000000			
9	Ge	4.238717	4.045963	2.739688	0.000000		
10	Ge	2.481353	4.169676	5.493574	4.169676	0.000000	
11	Ge	4.521282	4.055154	2.734544	2.504649	5.196135	0.000000



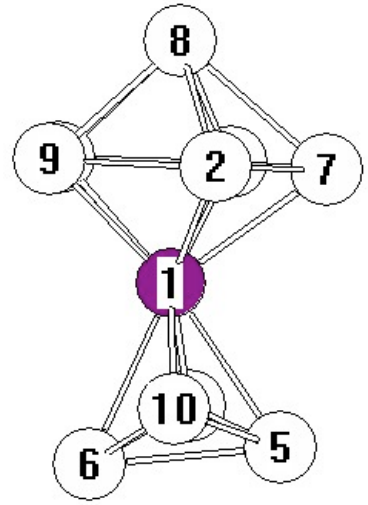
0-4 APT – C_{2v} [4] (ra-88) → C_s [4] [3]

- 21900.8739732 (+42.40 kcal/mol) ** i -13 **

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.745425	0.000000				
3	Ge	2.629318	5.297910	0.000000			
4	Ge	2.745277	4.063428	3.492762	0.000000		
5	Ge	2.794193	4.566341	2.467481	4.567685	0.000000	
6	Ge	2.804709	5.078979	2.476813	5.071934	2.712636	
7	Ge	2.733051	2.501280	4.398224	2.501632	3.989519	
8	Ge	3.432555	2.746789	5.539714	2.747430	5.926136	
9	Ge	2.722599	2.510091	5.097129	4.064060	5.343138	
10	Ge	2.628725	3.501625	3.899548	5.299408	2.467181	
11	Ge	2.722439	4.063692	4.020491	2.509973	5.343885	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	5.353525	0.000000				
8	Ge	6.123730	2.758864	0.000000			
9	Ge	4.541341	4.046851	2.727697	0.000000		
10	Ge	2.476699	4.407029	5.543357	4.018623	0.000000	
11	Ge	4.536664	4.046686	2.727618	2.513844	5.092987	0.000000



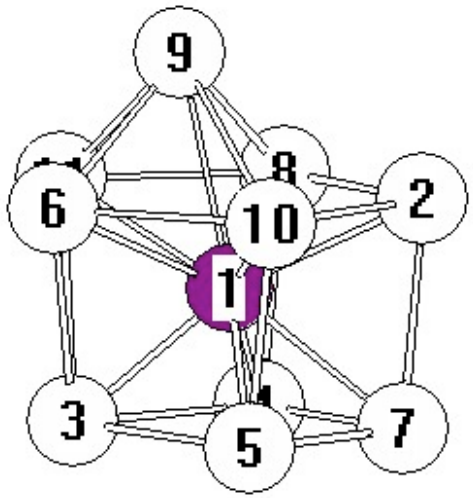
0-4 APT – C_{2v} [4] (ra-88, r-13) → C_1 [4] [2]

- 21900.8743482 (+42.17 kcal/mol)

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.439067	0.000000				
3	Ge	2.375927	4.772676	0.000000			
4	Ge	2.463078	3.755703	2.795669	0.000000		
5	Ge	2.463078	3.755703	2.795669	3.731214	0.000000	
6	Ge	2.635375	4.401926	2.962689	4.753311	3.535791	
7	Ge	2.542476	2.650728	3.784017	2.525295	2.525295	
8	Ge	2.495231	2.753346	4.133240	2.669681	4.849625	
9	Ge	2.768473	3.240496	4.426378	4.757050	4.757050	
10	Ge	2.495231	2.753346	4.133240	4.849625	2.669681	
11	Ge	2.635375	4.401926	2.962689	3.535791	4.753311	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.972718	0.000000				
8	Ge	4.357821	3.727596	0.000000			
9	Ge	2.538488	5.005828	2.970664	0.000000		
10	Ge	2.666111	3.727596	4.393117	2.970664	0.000000	
11	Ge	2.704788	4.972718	2.666111	2.538488	4.357821	0.000000



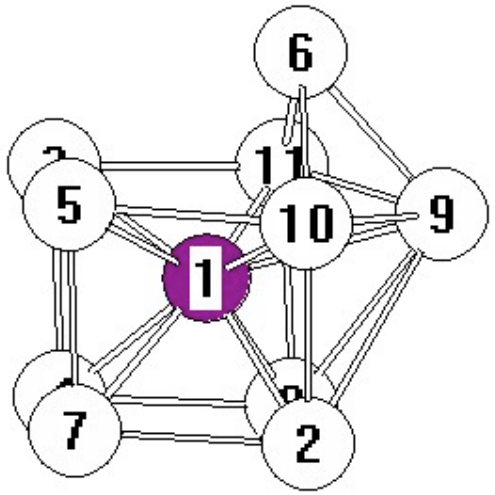
0-4 APT – C_{2v} [4] (rc-57) → C_s [4] [5]

- 21900.8706220 (+44.51 kcal/mol) ** i -49 **

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.432364	0.000000				
3	Ge	2.415371	4.776603	0.000000			
4	Ge	2.522549	3.734033	2.631024	0.000000		
5	Ge	2.417233	3.860213	2.806794	3.726832	0.000000	
6	Ge	2.777337	4.472033	3.381734	5.028372	3.391332	
7	Ge	2.525381	2.638165	3.726428	2.485285	2.627149	
8	Ge	2.430868	2.804370	3.871907	2.642943	4.776967	
9	Ge	2.765157	3.213038	4.546439	4.957806	4.550122	
10	Ge	2.549909	2.730761	4.421545	4.925749	2.747217	
11	Ge	2.550931	4.418289	2.750134	3.687527	4.430096	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	5.033537	0.000000				
8	Ge	4.467625	3.733811	0.000000			
9	Ge	2.449373	4.962584	3.202908	0.000000		
10	Ge	2.685749	3.693332	4.410197	2.726254	0.000000	
11	Ge	2.683778	4.927918	2.733035	2.724466	4.287006	0.000000



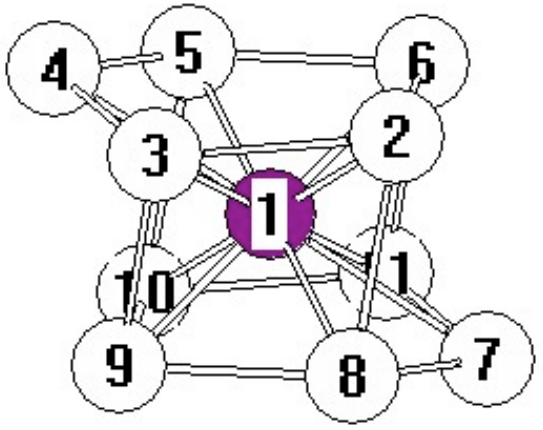
0-4 APT – C_{2v} [4] (rc-57, r-49) → C_1 [4] [4]

- 21900.8728911 (+43.08 kcal/mol)

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.491317	0.000000				
3	Ge	2.630392	2.636657	0.000000			
4	Ge	2.825841	4.139465	2.468137	0.000000		
5	Ge	2.630210	4.393553	4.153070	2.469044	0.000000	
6	Ge	2.491923	2.974088	4.393870	4.140219	2.637091	
7	Ge	2.825841	3.353938	4.870008	5.651682	4.869352	
8	Ge	2.630210	2.635531	3.228923	4.869352	5.260420	
9	Ge	2.491923	3.998435	2.636512	3.353910	4.393305	
10	Ge	2.491317	4.982634	4.393095	3.353938	2.635531	
11	Ge	2.630392	4.393095	5.260784	4.870008	3.228923	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.353910	0.000000				
8	Ge	4.393305	2.469044	0.000000			
9	Ge	4.983846	4.140219	2.637091	0.000000		
10	Ge	3.998435	4.139465	4.393553	2.974088	0.000000	
11	Ge	2.636512	2.468137	4.153070	4.393870	2.636657	0.000000



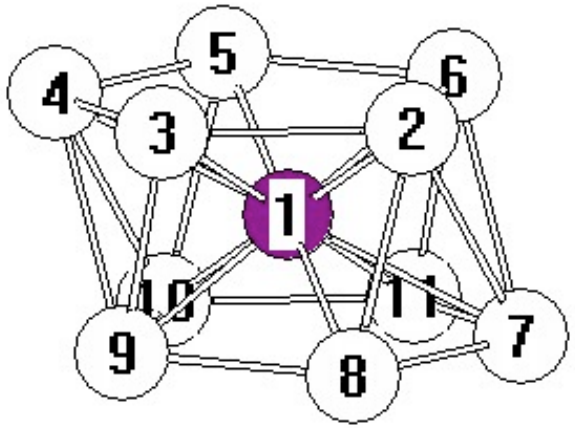
0-5 APP – C_{2h} [4] (ra-148) → C_i [4] [8]

- 21900.8592978 (+51.61 kcal/mol) ** i -49 **

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.455905	0.000000				
3	Ge	2.598836	2.701206	0.000000			
4	Ge	2.855770	4.366192	2.503861	0.000000		
5	Ge	2.597229	4.250468	3.972784	2.504741	0.000000	
6	Ge	2.455766	2.711394	4.251787	4.368147	2.702608	
7	Ge	2.855770	3.051254	4.852774	5.711540	4.850599	
8	Ge	2.597229	2.736359	3.349041	4.850599	5.194458	
9	Ge	2.455766	4.095467	2.737110	3.048231	4.271847	
10	Ge	2.455905	4.911810	4.274847	3.051254	2.736359	
11	Ge	2.598836	4.274847	5.197671	4.852774	3.349041	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.048231	0.000000				
8	Ge	4.271847	2.504741	0.000000			
9	Ge	4.911532	4.368147	2.702608	0.000000		
10	Ge	4.095467	4.366192	4.250468	2.711394	0.000000	
11	Ge	2.737110	2.503861	3.972784	4.251787	2.701206	0.000000



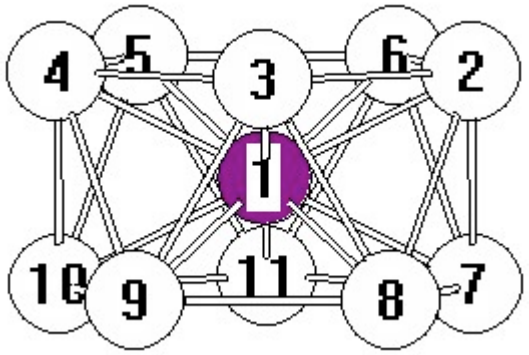
0-5 APP – C_{2h} [4] (rb-83) → C_i [4] [9]

- 21900.8557207 (+53.86 kcal/mol) ** i -44 **

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.598871	0.000000				
3	Ge	2.598871	2.719131	0.000000			
4	Ge	2.598871	4.399646	2.719131	0.000000		
5	Ge	2.598871	4.399646	4.399646	2.719131	0.000000	
6	Ge	2.598871	2.719131	4.399646	4.399646	2.719131	
7	Ge	2.598871	2.767603	4.429768	5.197741	4.429768	
8	Ge	2.598871	2.767603	2.767603	4.429768	5.197741	
9	Ge	2.598871	4.429768	2.767603	2.767603	4.429768	
10	Ge	2.598871	5.197741	4.429768	2.767603	2.767603	
11	Ge	2.598871	4.429768	5.197741	4.429768	2.767603	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.767603	0.000000				
8	Ge	4.429768	2.719131	0.000000			
9	Ge	5.197741	4.399646	2.719131	0.000000		
10	Ge	4.429768	4.399646	4.399646	2.719131	0.000000	
11	Ge	2.767603	2.719131	4.399646	4.399646	2.719131	0.000000



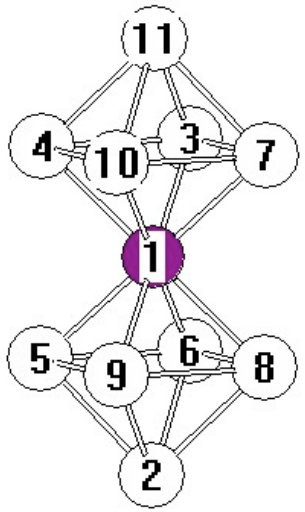
0-5 APP – D_{5d} [6] **[12]**

- 21900.8460873 (+59.90 kcal/mol)

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.530916	0.000000				
3	Ge	2.544429	5.573834	0.000000			
4	Ge	2.544429	5.573834	2.655393	0.000000		
5	Ge	2.544429	2.610621	4.341125	3.434277	0.000000	
6	Ge	2.544429	2.610621	3.434277	4.341125	2.655393	
7	Ge	2.544429	5.573834	2.655393	3.755292	5.088858	
8	Ge	2.544429	2.610621	4.341125	5.088858	3.755292	
9	Ge	2.544429	2.610621	5.088858	4.341125	2.655393	
10	Ge	2.544429	5.573834	3.755292	2.655393	4.341125	
11	Ge	3.530916	7.061831	2.610621	2.610621	5.573834	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.341125	0.000000				
8	Ge	2.655393	3.434277	0.000000			
9	Ge	3.755292	4.341125	2.655393	0.000000		
10	Ge	5.088858	2.655393	4.341125	3.434277	0.000000	
11	Ge	5.573834	2.610621	5.573834	5.573834	2.610621	0.000000



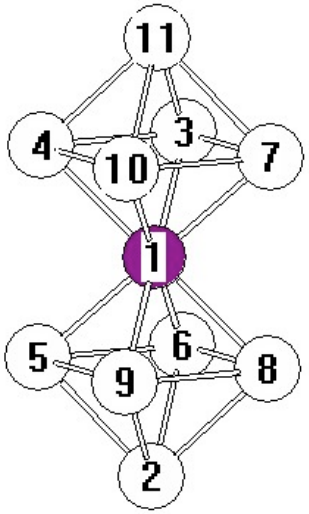
0-8 CBO – D_{4h} [2] **[6]**

- 21900.8618024 (+50.04 kcal/mol)

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.524289	0.000000				
3	Ge	2.531503	5.552220	0.000000			
4	Ge	2.531503	5.552220	2.649927	0.000000		
5	Ge	2.531503	2.613638	4.314153	3.404380	0.000000	
6	Ge	2.531503	2.613638	3.404380	4.314153	2.649927	
7	Ge	2.531503	5.552220	2.649927	3.747562	5.063006	
8	Ge	2.531503	2.613638	4.314153	5.063006	3.747562	
9	Ge	2.531503	2.613638	5.063006	4.314153	2.649927	
10	Ge	2.531503	5.552220	3.747562	2.649927	4.314153	
11	Ge	3.524289	7.048579	2.613638	2.613638	5.552220	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.314153	0.000000				
8	Ge	2.649927	3.404380	0.000000			
9	Ge	3.747562	4.314153	2.649927	0.000000		
10	Ge	5.063006	2.649927	4.314153	3.404380	0.000000	
11	Ge	5.552220	2.613638	5.552220	5.552220	2.613638	0.000000



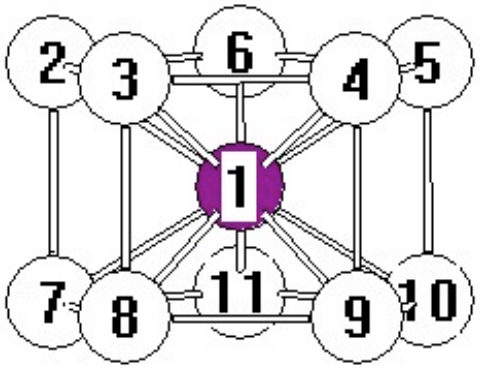
0-8 CBO – D_{4h} [4] [7]

- 21900.8616066 (+50.16 kcal/mol)

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.540823	0.000000				
3	Ge	2.540790	2.555599	0.000000			
4	Ge	2.540772	4.134981	2.555526	0.000000		
5	Ge	2.540783	4.134958	4.134970	2.555577	0.000000	
6	Ge	2.540839	2.555526	4.134996	4.135006	2.555569	
7	Ge	2.540823	2.630549	3.667561	4.900794	4.900741	
8	Ge	2.540790	3.667561	2.630597	3.667499	4.900763	
9	Ge	2.540772	4.900794	3.667499	2.630520	3.667462	
10	Ge	2.540783	4.900741	4.900763	3.667462	2.630393	
11	Ge	2.540839	3.667450	4.900795	4.900783	3.667424	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.667450	0.000000				
8	Ge	4.900795	2.555599	0.000000			
9	Ge	4.900783	4.134981	2.555526	0.000000		
10	Ge	3.667424	4.134958	4.134970	2.555577	0.000000	
11	Ge	2.630430	2.555526	4.134996	4.135006	2.555569	0.000000



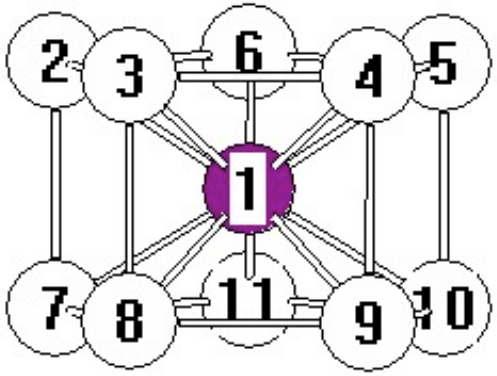
0-9 PPG – C_s [2] [1]

- 21900.9415464 (**+0.00 kcal/mol**)

Charge 4-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.541375	0.000000				
3	Ge	2.541364	2.555708	0.000000			
4	Ge	2.541304	4.135176	2.555668	0.000000		
5	Ge	2.541304	4.135176	4.135218	2.555737	0.000000	
6	Ge	2.541364	2.555708	4.135240	4.135218	2.555668	
7	Ge	2.541375	2.632019	3.668712	4.901847	4.901847	
8	Ge	2.541364	3.668712	2.632126	3.668807	4.901911	
9	Ge	2.541304	4.901847	3.668807	2.632361	3.668940	
10	Ge	2.541304	4.901847	4.901911	3.668940	2.632361	
11	Ge	2.541364	3.668712	4.901867	4.901911	3.668807	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.668712	0.000000				
8	Ge	4.901867	2.555708	0.000000			
9	Ge	4.901911	4.135176	2.555668	0.000000		
10	Ge	3.668807	4.135176	4.135218	2.555737	0.000000	
11	Ge	2.632126	2.555708	4.135240	4.135218	2.555668	0.000000



0-9 PPG – C_{2v} [2] [1]

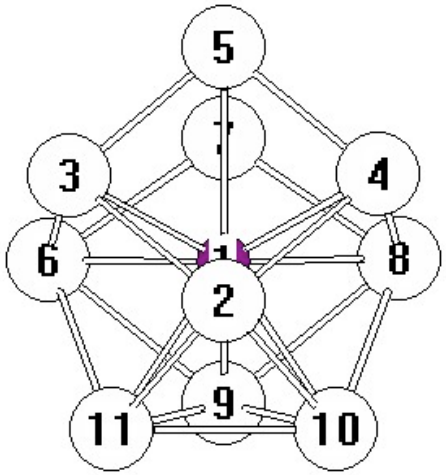
- 21900.9414750 (**+0.04 kcal/mol**)

$Mn@Ge_{10}^{3-}$

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.408584	0.000000				
3	Ge	2.413489	2.624118	0.000000			
4	Ge	2.413489	2.624118	3.647547	0.000000		
5	Ge	2.551841	3.606936	2.513517	2.513517	0.000000	
6	Ge	2.409091	4.165383	2.624097	4.699133	3.607852	
7	Ge	2.412969	4.698021	3.646776	3.646776	2.513537	
8	Ge	2.409091	4.165383	4.699133	2.624097	3.607852	
9	Ge	2.438966	4.311709	4.412991	4.412991	4.706727	
10	Ge	2.438945	2.748150	4.413217	3.132059	4.706800	
11	Ge	2.438945	2.748150	3.132059	4.413217	4.706800	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.624273	0.000000				
8	Ge	4.166077	2.624273	0.000000			
9	Ge	2.747833	3.131305	2.747833	0.000000		
10	Ge	4.311651	4.412460	2.747625	2.650207	0.000000	
11	Ge	2.747625	4.412460	4.311651	2.650207	2.650189	0.000000



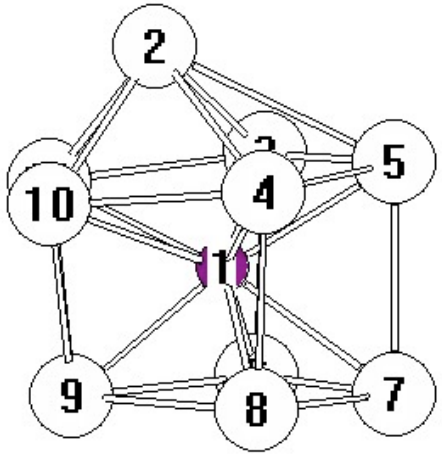
0-3 CCD – C_1 [1] **[7]**

- 21901.1920573 (+23.39 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.741956	0.000000				
3	Ge	2.495806	2.928446	0.000000			
4	Ge	2.495806	2.928446	4.340925	0.000000		
5	Ge	2.374764	3.140483	2.662994	2.662994	0.000000	
6	Ge	2.431580	4.673717	2.632334	4.827242	3.691812	
7	Ge	2.510995	4.988048	3.736794	3.736794	2.736999	
8	Ge	2.431580	4.673717	4.827242	2.632334	3.691812	
9	Ge	2.339203	4.252615	4.105830	4.105830	4.700254	
10	Ge	2.615849	2.532745	4.355544	2.660218	4.303491	
11	Ge	2.615849	2.532745	2.660218	4.355544	4.303491	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.486697	0.000000				
8	Ge	3.771797	2.486697	0.000000			
9	Ge	2.883695	3.802143	2.883695	0.000000		
10	Ge	4.711266	4.904921	3.444040	2.781672	0.000000	
11	Ge	3.444040	4.904921	4.711266	2.781672	2.739970	0.000000



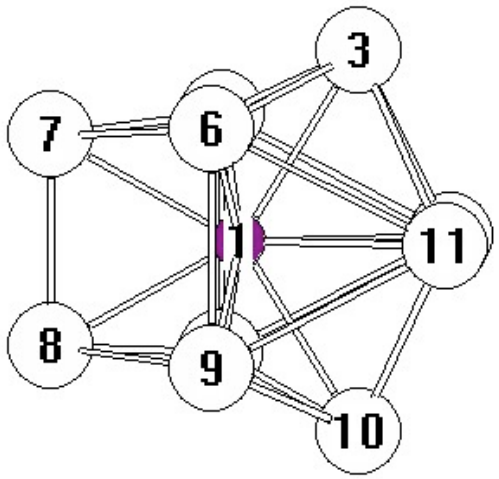
0-3 CCD – C_s [3] **[6]**

- 21901.1930015 (+22.80 kcal/mol) ** i -15 **

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.705510	0.000000				
3	Ge	2.574967	2.713477	0.000000			
4	Ge	2.374491	3.084545	4.358001	0.000000		
5	Ge	2.373245	3.081068	2.652158	2.738554	0.000000	
6	Ge	2.373722	4.361323	2.651289	4.716642	3.837581	
7	Ge	2.495081	4.902663	3.680725	3.739989	2.713207	
8	Ge	2.495243	4.903109	4.910411	2.711686	3.740530	
9	Ge	2.372897	4.360935	4.355219	3.840434	4.715088	
10	Ge	2.573382	2.713668	4.360540	2.652375	4.354310	
11	Ge	2.706979	2.468211	2.710811	4.359657	4.356619	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.710377	0.000000				
8	Ge	3.740554	2.421781	0.000000			
9	Ge	2.739189	3.739506	2.713314	0.000000		
10	Ge	4.357371	4.908656	3.679504	2.652662	0.000000	
11	Ge	3.092652	4.906615	4.907368	3.090630	2.712403	0.000000



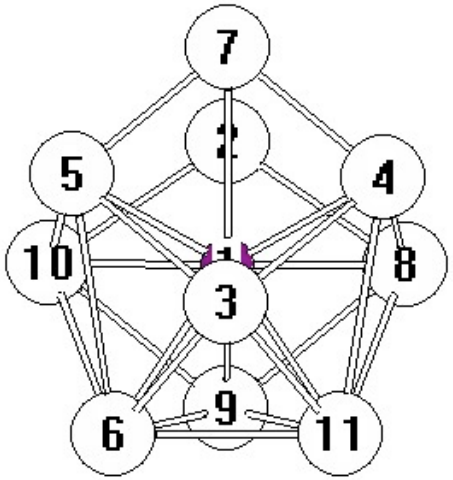
0-3 CCD – C_s [3] (r-15) → C_1 [3] [5]

- 21901.1936351 (+22.40 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.411215	0.000000				
3	Ge	2.407157	4.696528	0.000000			
4	Ge	2.410252	3.646867	2.626365	0.000000		
5	Ge	2.417376	3.645591	2.623670	3.642470	0.000000	
6	Ge	2.441308	4.411576	2.744743	4.411078	3.149726	
7	Ge	2.553682	2.514250	3.611972	2.514141	2.509973	
8	Ge	2.411796	2.626762	4.169566	2.626134	4.703915	
9	Ge	2.439715	3.129162	4.308701	4.408967	4.422568	
10	Ge	2.405579	2.626355	4.153243	4.693698	2.624803	
11	Ge	2.439612	4.409912	2.749619	3.126645	4.420960	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.714401	0.000000				
8	Ge	4.311323	3.611064	0.000000			
9	Ge	2.648277	4.708692	2.744911	0.000000		
10	Ge	2.743501	3.609484	4.169115	2.751545	0.000000	
11	Ge	2.650163	4.707904	2.744253	2.648679	4.309026	0.000000



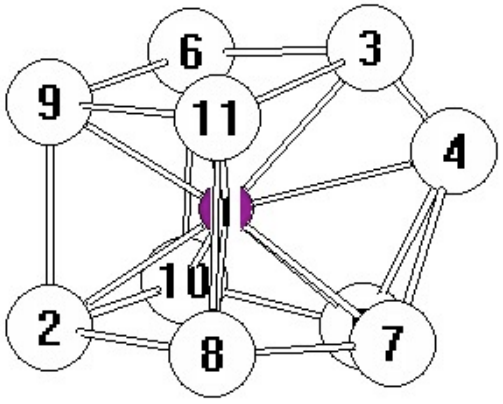
0-4 APT – D_{4d} [1] (r-67) → C_1 [1] [7]

- 21901.1920504 (+23.39 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.419786	0.000000				
3	Ge	2.488300	4.868734	0.000000			
4	Ge	2.644938	4.521534	2.779787	0.000000		
5	Ge	2.644938	4.521534	2.779787	2.612132	0.000000	
6	Ge	2.419885	3.829504	2.724890	4.524537	3.235393	
7	Ge	2.644276	3.229818	4.339259	2.611584	2.611584	
8	Ge	2.488233	2.722313	4.252259	2.778102	4.338618	
9	Ge	2.396358	2.626296	3.725522	4.811892	4.811892	
10	Ge	2.488233	2.722313	4.252259	4.338618	2.778102	
11	Ge	2.419885	3.829504	2.724890	3.235393	4.524537	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.522979	0.000000				
8	Ge	4.868215	2.777642	0.000000			
9	Ge	2.622707	4.810656	3.725530	0.000000		
10	Ge	2.723448	2.777642	4.251604	3.725530	0.000000	
11	Ge	3.829694	4.522979	2.723448	2.622707	4.868215	0.000000



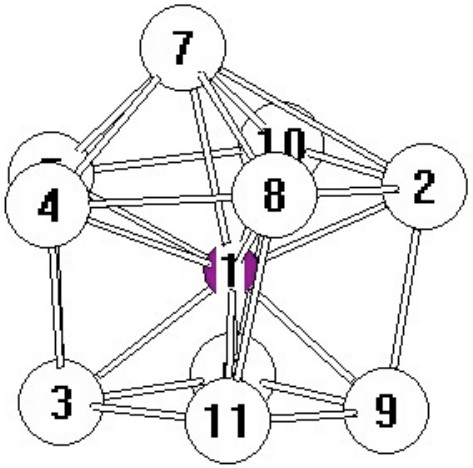
0-4 APT – C_{2v} [5] (ra-59) → C_s [5] [8]

- 21901.1853920 (+27.57 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.423088	0.000000				
3	Ge	2.484028	4.870146	0.000000			
4	Ge	2.643860	4.510919	2.787801	0.000000		
5	Ge	2.643860	4.510919	2.787801	2.612978	0.000000	
6	Ge	2.417855	3.835142	2.723075	4.528337	3.243379	
7	Ge	2.651628	3.214865	4.346671	2.610470	2.610470	
8	Ge	2.490116	2.722280	4.248688	2.767386	4.333328	
9	Ge	2.395791	2.626814	3.734822	4.815242	4.815242	
10	Ge	2.490116	2.722280	4.248688	4.333328	2.767386	
11	Ge	2.417855	3.835142	2.723075	3.243379	4.528337	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.530875	0.000000				
8	Ge	4.867823	2.778019	0.000000			
9	Ge	2.624519	4.808279	3.722787	0.000000		
10	Ge	2.726221	2.778019	4.255415	3.722787	0.000000	
11	Ge	3.821818	4.530875	2.726221	2.624519	4.867823	0.000000



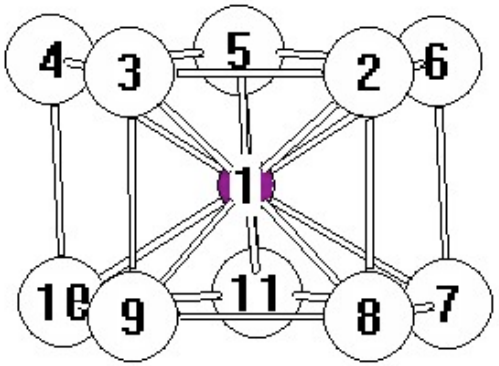
0-4 APT – C_{2v} [5] (rb-35) → C_s [5] [9]

- 21901.1853855 (+27.57 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.464173	0.000000				
3	Ge	2.482977	2.552810	0.000000			
4	Ge	2.557536	4.112935	2.537432	0.000000		
5	Ge	2.606243	4.116144	4.119719	2.546171	0.000000	
6	Ge	2.542394	2.554286	4.135039	4.123295	2.545432	
7	Ge	2.606243	3.576148	4.896228	4.987826	3.805432	
8	Ge	2.557536	2.613309	3.662410	4.942387	4.987826	
9	Ge	2.482977	3.635553	2.618761	3.662410	4.896228	
10	Ge	2.464173	4.798570	3.635553	2.613309	3.576148	
11	Ge	2.542394	4.765021	4.875882	3.726274	2.617373	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.617373	0.000000				
8	Ge	3.726274	2.546171	0.000000			
9	Ge	4.875882	4.119719	2.537432	0.000000		
10	Ge	4.765021	4.116144	4.112935	2.552810	0.000000	
11	Ge	3.487003	2.545432	4.123295	4.135039	2.554286	0.000000



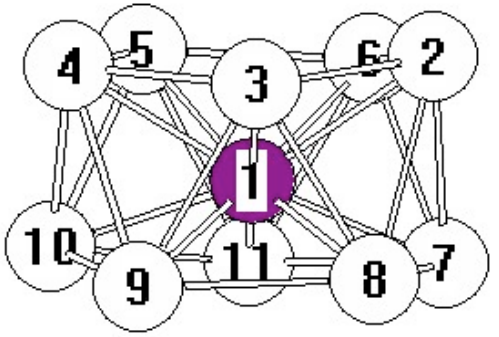
0-5 APP – D_{5d} [3] (ra-79) → C_2 [3] [1]

- 21901.2293295 (+0.00 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.606761	0.000000				
3	Ge	2.706857	2.705922	0.000000			
4	Ge	2.658958	4.183631	2.621719	0.000000		
5	Ge	2.658958	4.183631	4.491044	2.910061	0.000000	
6	Ge	2.706857	2.705922	4.569001	4.491044	2.621719	
7	Ge	2.548498	2.830295	4.464450	5.193480	4.345179	
8	Ge	2.548498	2.830295	2.688278	4.345179	5.193480	
9	Ge	2.551582	4.413044	2.741293	2.771351	4.527366	
10	Ge	2.524974	5.086165	4.382626	2.689508	2.689508	
11	Ge	2.551582	4.413044	5.257161	4.527366	2.771351	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.688278	0.000000				
8	Ge	4.464450	2.780581	0.000000			
9	Ge	5.257161	4.427608	2.712438	0.000000		
10	Ge	4.382626	4.506301	4.506301	2.793189	0.000000	
11	Ge	2.741293	2.712438	4.427608	4.404257	2.793189	0.000000



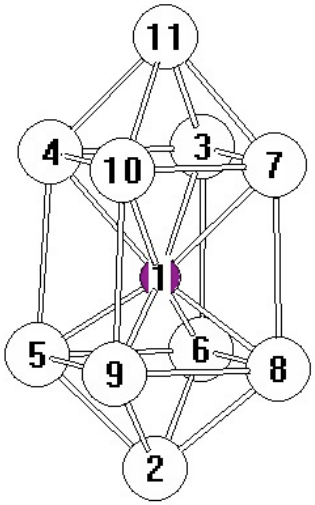
0-5 APP – C_{2h} [7] (r-92) → C_s [7] [11]

- 21901.1224564 (+67.06 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.956868	0.000000				
3	Ge	2.580637	5.117569	0.000000			
4	Ge	2.580637	5.117569	2.581724	0.000000		
5	Ge	2.357332	2.564721	4.120726	3.132838	0.000000	
6	Ge	2.357332	2.564721	3.132838	4.120726	2.775551	
7	Ge	2.580637	5.117569	2.581724	3.651109	4.913867	
8	Ge	2.357332	2.564721	4.120726	4.913867	3.925223	
9	Ge	2.357332	2.564721	4.913867	4.120726	2.775551	
10	Ge	2.580637	5.117569	3.651109	2.581724	4.120726	
11	Ge	3.705945	6.662812	2.621888	2.621888	5.382346	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.120726	0.000000				
8	Ge	2.775551	3.132838	0.000000			
9	Ge	3.925223	4.120726	2.775551	0.000000		
10	Ge	4.913867	2.581724	4.120726	3.132838	0.000000	
11	Ge	5.382346	2.621888	5.382346	5.382346	2.621888	0.000000



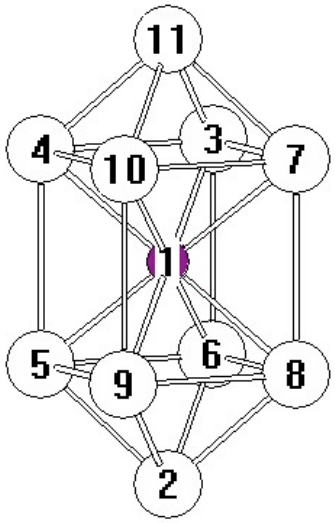
0-8 CBO – D_{4h} [1] (r-256) → C_{4v} [1] [12]

- 21901.1121493 (+73.53 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.229128	0.000000				
3	Ge	2.487889	5.166682	0.000000			
4	Ge	2.487889	5.166682	2.740295	0.000000		
5	Ge	2.487889	2.557170	4.153210	3.120887	0.000000	
6	Ge	2.487889	2.557170	3.120887	4.153210	2.740295	
7	Ge	2.487889	5.166682	2.740295	3.875362	4.975778	
8	Ge	2.487889	2.557170	4.153210	4.975778	3.875362	
9	Ge	2.487889	2.557170	4.975778	4.153210	2.740295	
10	Ge	2.487889	5.166682	3.875362	2.740295	4.153210	
11	Ge	3.229128	6.458256	2.557170	2.557170	5.166682	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.153210	0.000000				
8	Ge	2.740295	3.120887	0.000000			
9	Ge	3.875362	4.153210	2.740295	0.000000		
10	Ge	4.975778	2.740295	4.153210	3.120887	0.000000	
11	Ge	5.166682	2.557170	5.166682	5.166682	2.557170	0.000000



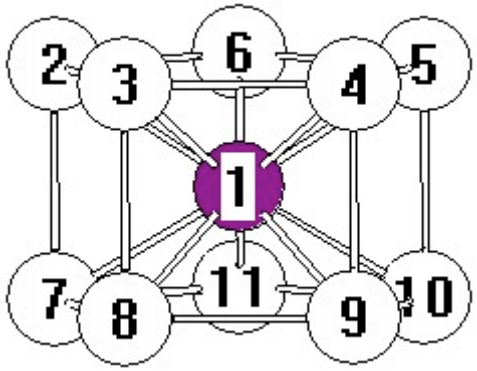
0-8 CBO – D_{4h} [3] [10]

- 21901.1657038 (+39.93 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.515404	0.000000				
3	Ge	2.515404	2.531389	0.000000			
4	Ge	2.515404	4.095874	2.531389	0.000000		
5	Ge	2.515404	4.095874	4.095874	2.531389	0.000000	
6	Ge	2.515404	2.531389	4.095874	4.095874	2.531389	
7	Ge	2.515404	2.600333	3.629003	4.851589	4.851589	
8	Ge	2.515404	3.629003	2.600333	3.629003	4.851589	
9	Ge	2.515404	4.851589	3.629003	2.600333	3.629003	
10	Ge	2.515404	4.851589	4.851589	3.629003	2.600333	
11	Ge	2.515404	3.629003	4.851589	4.851589	3.629003	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.629003	0.000000				
8	Ge	4.851589	2.531389	0.000000			
9	Ge	4.851589	4.095874	2.531389	0.000000		
10	Ge	3.629003	4.095874	4.095874	2.531389	0.000000	
11	Ge	2.600333	2.531389	4.095874	4.095874	2.531389	0.000000



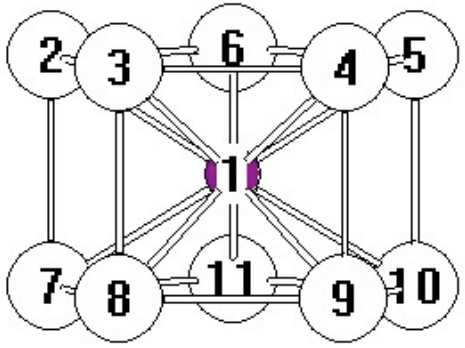
0-9 PPG – D_{5h} [1] [4]

- 21901.2062175 (+14.50 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.514952	0.000000				
3	Ge	2.514914	2.531430	0.000000			
4	Ge	2.514872	4.095968	2.531408	0.000000		
5	Ge	2.514872	4.095968	4.095914	2.531442	0.000000	
6	Ge	2.514914	2.531430	4.095882	4.095914	2.531408	
7	Ge	2.514952	2.598073	3.627506	4.850543	4.850543	
8	Ge	2.514914	3.627506	2.598333	3.627605	4.850568	
9	Ge	2.514872	4.850543	3.627605	2.598393	3.627650	
10	Ge	2.514872	4.850543	4.850568	3.627650	2.598393	
11	Ge	2.514914	3.627506	4.850524	4.850568	3.627605	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.627506	0.000000				
8	Ge	4.850524	2.531430	0.000000			
9	Ge	4.850568	4.095968	2.531408	0.000000		
10	Ge	3.627605	4.095968	4.095914	2.531442	0.000000	
11	Ge	2.598333	2.531430	4.095882	4.095914	2.531408	0.000000



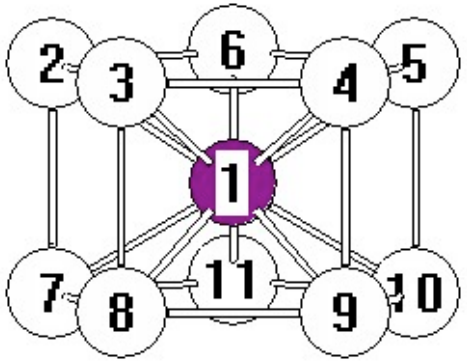
0-9 PPG – C_s [1] [4]

- 21901.2061829 (+14.52 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.516044	0.000000				
3	Ge	2.516079	2.532074	0.000000			
4	Ge	2.516043	4.096972	2.532077	0.000000		
5	Ge	2.516044	4.096988	4.096998	2.532073	0.000000	
6	Ge	2.516023	2.532094	4.096998	4.096968	2.532060	
7	Ge	2.516044	2.600922	3.629872	4.852793	4.852846	
8	Ge	2.516079	3.629872	2.600838	3.629823	4.852832	
9	Ge	2.516043	4.852793	3.629823	2.600776	3.629852	
10	Ge	2.516044	4.852846	4.852832	3.629852	2.600927	
11	Ge	2.516023	3.629932	4.852843	4.852801	3.629911	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.629932	0.000000				
8	Ge	4.852843	2.532074	0.000000			
9	Ge	4.852801	4.096972	2.532077	0.000000		
10	Ge	3.629911	4.096988	4.096998	2.532073	0.000000	
11	Ge	2.600966	2.532094	4.096998	4.096968	2.532060	0.000000



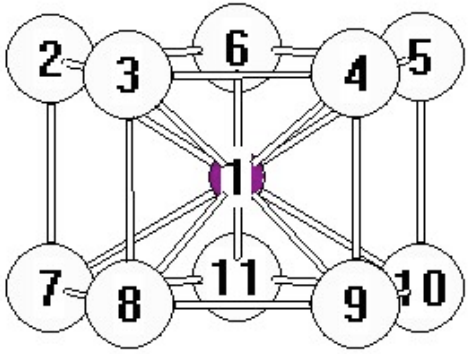
0-9 PPG – C_s [1] **[4]**

- 21901.2062275 (+14.50 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.526772	0.000000				
3	Ge	2.521193	2.583827	0.000000			
4	Ge	2.507807	4.123149	2.526353	0.000000		
5	Ge	2.507807	4.123149	4.090837	2.496532	0.000000	
6	Ge	2.521193	2.583827	4.146749	4.090837	2.526353	
7	Ge	2.526772	2.552764	3.637731	4.858237	4.858237	
8	Ge	2.521193	3.637731	2.568561	3.609075	4.835072	
9	Ge	2.507807	4.858237	3.609075	2.586260	3.594637	
10	Ge	2.507807	4.858237	4.835072	3.594637	2.586260	
11	Ge	2.521193	3.637731	4.877810	4.835072	3.609075	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.637731	0.000000				
8	Ge	4.877810	2.583827	0.000000			
9	Ge	4.835072	4.123149	2.526353	0.000000		
10	Ge	3.609075	4.123149	4.090837	2.496532	0.000000	
11	Ge	2.568561	2.583827	4.146749	4.090837	2.526353	0.000000



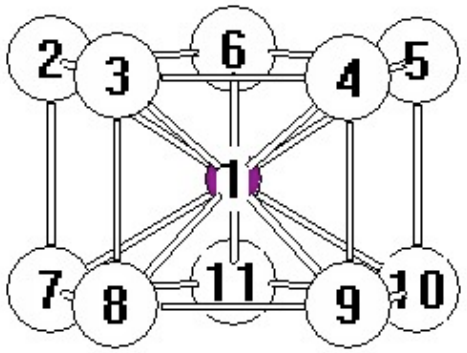
0-9 PPG – C_{2v} [3] **[3]**

- 21901.2290832 (+0.15 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.511865	0.000000				
3	Ge	2.524499	2.546781	0.000000			
4	Ge	2.525524	4.134833	2.594430	0.000000		
5	Ge	2.516205	4.085422	4.143366	2.565117	0.000000	
6	Ge	2.505546	2.499240	4.099424	4.109632	2.510076	
7	Ge	2.511865	2.581462	3.619028	4.867770	4.831230	
8	Ge	2.524499	3.619028	2.561058	3.643796	4.874940	
9	Ge	2.525524	4.867770	3.643796	2.556047	3.628287	
10	Ge	2.516205	4.831230	4.874940	3.628287	2.576105	
11	Ge	2.505546	3.594995	4.840484	4.847795	3.600612	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.594995	0.000000				
8	Ge	4.840484	2.546781	0.000000			
9	Ge	4.847795	4.134833	2.594430	0.000000		
10	Ge	3.600612	4.085422	4.143366	2.565117	0.000000	
11	Ge	2.586823	2.499240	4.099424	4.109632	2.510076	0.000000



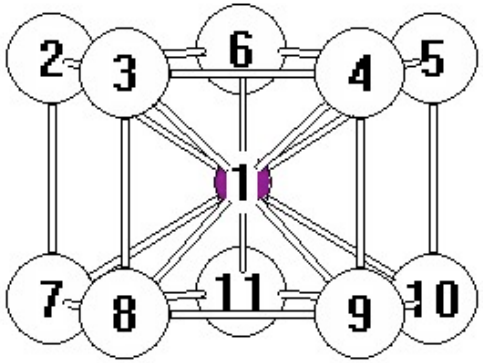
0-9 PPG – C_s [7] (r-16, r-17, r-13) → C_s [3] [2]

- 21901.2291593 (+0.11 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.515530	0.000000				
3	Ge	2.515365	2.531499	0.000000			
4	Ge	2.515397	4.096161	2.531617	0.000000		
5	Ge	2.515558	4.096091	4.096120	2.531555	0.000000	
6	Ge	2.515627	2.531524	4.096072	4.096117	2.531488	
7	Ge	2.515530	2.600219	3.629109	4.851819	4.851708	
8	Ge	2.515365	3.629109	2.600529	3.629257	4.851815	
9	Ge	2.515397	4.851819	3.629257	2.600404	3.629098	
10	Ge	2.515558	4.851708	4.851815	3.629098	2.600205	
11	Ge	2.515627	3.628938	4.851720	4.851725	3.628907	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.628938	0.000000				
8	Ge	4.851720	2.531499	0.000000			
9	Ge	4.851725	4.096161	2.531617	0.000000		
10	Ge	3.628907	4.096091	4.096120	2.531555	0.000000	
11	Ge	2.600002	2.531524	4.096072	4.096117	2.531488	0.000000



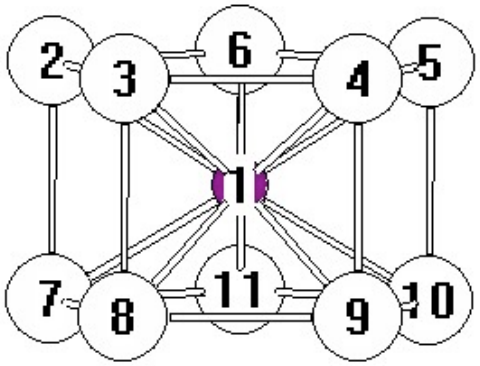
0-9 PPG – C_s [7] (r-16, r-17) → C_s [1] [4]

- 21901.2062720 (+14.47 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.517216	0.000000				
3	Ge	2.512515	2.531756	0.000000			
4	Ge	2.516808	4.101177	2.532306	0.000000		
5	Ge	2.517370	4.100319	4.094070	2.530761	0.000000	
6	Ge	2.513907	2.531917	4.091261	4.094966	2.531714	
7	Ge	2.517216	2.600208	3.629652	4.855571	4.855178	
8	Ge	2.512515	3.629652	2.601555	3.629462	4.850263	
9	Ge	2.516808	4.855571	3.629462	2.598610	3.627773	
10	Ge	2.517370	4.855178	4.850263	3.627773	2.599846	
11	Ge	2.513907	3.629314	4.848014	4.850351	3.629042	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.629314	0.000000				
8	Ge	4.848014	2.531756	0.000000			
9	Ge	4.850351	4.101177	2.532306	0.000000		
10	Ge	3.629042	4.100319	4.094070	2.530761	0.000000	
11	Ge	2.600298	2.531917	4.091261	4.094966	2.531714	0.000000



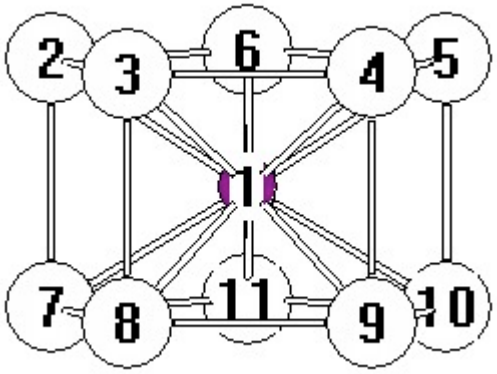
0-9 PPG – C_s [7] (r-16) → C_s [1] [4]

- 21901.2061894 (+14.52 kcal/mol)

Charge 3-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.573320	0.000000				
3	Ge	2.573277	2.594994	0.000000			
4	Ge	2.573196	4.198761	2.594939	0.000000		
5	Ge	2.573196	4.198761	4.198717	2.594951	0.000000	
6	Ge	2.573277	2.594994	4.198738	4.198717	2.594939	
7	Ge	2.573320	2.644773	3.705318	4.962383	4.962383	
8	Ge	2.573277	3.705318	2.644987	3.705391	4.962403	
9	Ge	2.573196	4.962383	3.705391	2.645084	3.705434	
10	Ge	2.573196	4.962383	4.962403	3.705434	2.645084	
11	Ge	2.573277	3.705318	4.962394	4.962403	3.705391	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.705318	0.000000				
8	Ge	4.962394	2.594994	0.000000			
9	Ge	4.962403	4.198761	2.594939	0.000000		
10	Ge	3.705391	4.198761	4.198717	2.594951	0.000000	
11	Ge	2.644987	2.594994	4.198738	4.198717	2.594939	0.000000



0-9 PPG – C_s [9] [13]

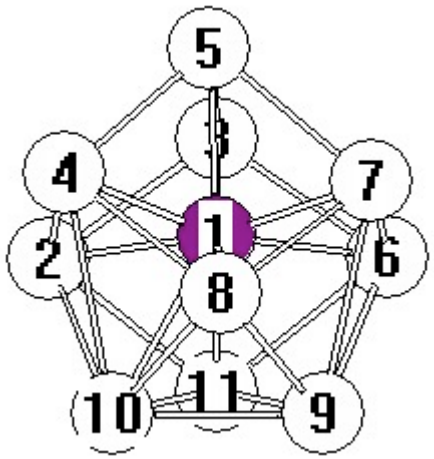
- 21901.0777834 (+95.10 kcal/mol)

$Mn@Ge_{10}^{2-}$

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.442573	0.000000				
3	Ge	2.408406	2.723950	0.000000			
4	Ge	2.408406	2.723950	3.883260	0.000000		
5	Ge	2.352812	3.618318	2.593923	2.593923	0.000000	
6	Ge	2.496981	4.221688	2.691422	4.872215	3.737528	
7	Ge	2.368078	4.793228	3.829885	3.829885	2.784545	
8	Ge	2.496981	4.221688	4.872215	2.691422	3.737528	
9	Ge	2.631115	4.276437	4.472705	4.472705	4.781913	
10	Ge	2.625037	2.721851	4.499660	3.153271	4.726579	
11	Ge	2.625037	2.721851	3.153271	4.499660	4.726579	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.641799	0.000000				
8	Ge	4.247650	2.641799	0.000000			
9	Ge	2.755645	3.047697	2.755645	0.000000		
10	Ge	4.339819	4.391689	2.750152	2.619932	0.000000	
11	Ge	2.750152	4.391689	4.339819	2.619932	2.653394	0.000000



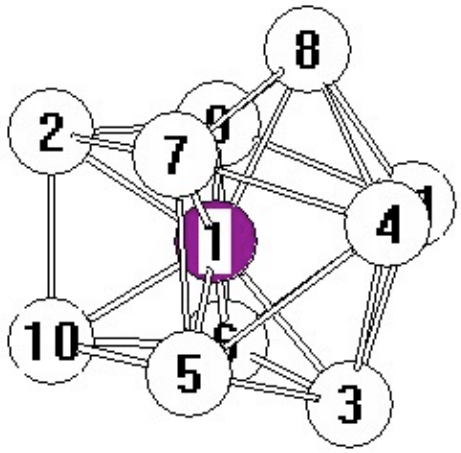
0-3 CCD – C_s [4] [4]

- 21901.3758516 (+8.12 kcal/mol) ** i -33 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.404736	0.000000				
3	Ge	2.557296	4.909508	0.000000			
4	Ge	2.640756	4.576988	2.725478	0.000000		
5	Ge	2.386142	3.849382	2.647297	3.017605	0.000000	
6	Ge	2.386142	3.849382	2.647297	4.372879	3.833461	
7	Ge	2.441599	2.753097	4.253021	2.757772	2.666581	
8	Ge	2.608182	3.309439	4.336534	2.641720	4.402317	
9	Ge	2.441599	2.753097	4.253021	4.305118	4.810928	
10	Ge	2.354971	2.540532	3.731918	4.744553	2.716011	
11	Ge	2.640756	4.576988	2.725478	2.612817	4.372879	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.810928	0.000000				
8	Ge	4.402317	2.728030	0.000000			
9	Ge	2.666581	4.182743	2.728030	0.000000		
10	Ge	2.716011	3.693699	4.759674	3.693699	0.000000	
11	Ge	3.017605	4.305118	2.641720	2.757772	4.744553	0.000000



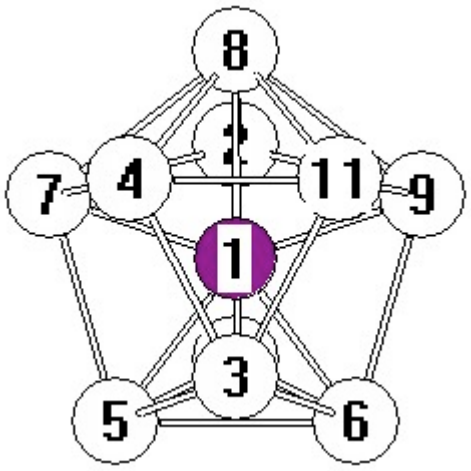
0-4 APT – D_{4d} [4] (rb-17) → C_s [4] [3]

- 21901.3760424 (+8.00 kcal/mol)

Charge 2-

		1	2	3	4	5	6
1	Mn	0.000000					
2	Ge	2.560923	0.000000				
3	Ge	2.661482	5.222319	0.000000			
4	Ge	2.636263	4.440302	2.731764	0.000000		
5	Ge	2.456504	4.291466	2.676617	3.583573	0.000000	
6	Ge	2.456504	4.291466	2.676617	4.505838	2.913153	
7	Ge	2.423439	2.925167	4.117869	2.677661	2.905307	
8	Ge	2.553737	2.659897	4.439264	2.724114	4.750416	
9	Ge	2.423439	2.925167	4.117869	4.330398	4.649296	
10	Ge	2.471379	2.621970	4.398116	4.940891	2.756749	
11	Ge	2.636263	4.440302	2.731764	2.560998	4.505838	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.649296	0.000000				
8	Ge	4.750416	2.942408	0.000000			
9	Ge	2.905307	4.522642	2.942408	0.000000		
10	Ge	2.756749	3.488749	4.466454	3.488749	0.000000	
11	Ge	3.583573	4.330398	2.724114	2.677661	4.940891	0.000000



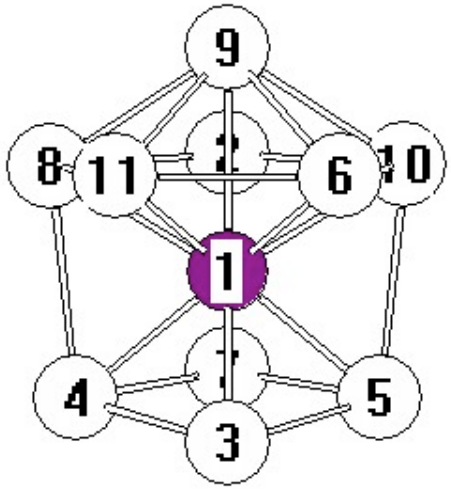
0-4 APT – C_{2v} [6] (ra-181) → C_s [6] [9]

- 21901.3176256 (+44.66 kcal/mol) ** i -52 **

Charge 2-

		1	2	3	4	5	6
1	Mn	0.000000					
2	Ge	2.750685	0.000000				
3	Ge	2.407486	5.003378	0.000000			
4	Ge	2.457116	3.900657	2.635279	0.000000		
5	Ge	2.457116	3.900657	2.635279	3.679922	0.000000	
6	Ge	2.469466	4.290756	3.536090	4.756530	3.557898	
7	Ge	2.568007	2.615867	3.610508	2.524630	2.524630	
8	Ge	2.625117	2.654934	4.468177	2.832016	4.880119	
9	Ge	2.696869	2.717956	4.911639	4.644937	4.644937	
10	Ge	2.625117	2.654934	4.468177	4.880119	2.832016	
11	Ge	2.469466	4.290756	3.536090	3.557898	4.756530	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.819861	0.000000				
8	Ge	4.306756	3.594456	0.000000			
9	Ge	2.637733	4.528672	2.704203	0.000000		
10	Ge	2.631318	3.594456	4.292277	2.704203	0.000000	
11	Ge	2.708193	4.819861	2.631318	2.637733	4.306756	0.000000



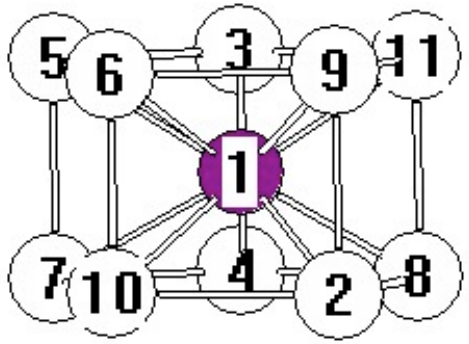
0-4 APT – C_{2v} [6] (rb-118) → C_s [6] [7]

- 21901.3367177 (+32.67 kcal/mol)

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.430624	0.000000				
3	Ge	2.606186	4.889555	0.000000			
4	Ge	2.598995	4.167677	2.523357	0.000000		
5	Ge	2.644123	4.897251	2.550365	3.597988	0.000000	
6	Ge	2.518103	3.628685	4.151459	4.850186	2.566890	
7	Ge	2.645175	4.191568	3.584332	2.553320	2.530307	
8	Ge	2.473176	2.586980	3.609698	2.580979	4.876579	
9	Ge	2.432946	2.557561	4.186605	4.888373	4.175226	
10	Ge	2.513535	2.590681	4.850283	4.131753	3.607388	
11	Ge	2.467061	3.629679	2.577998	3.616949	4.145916	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.598888	0.000000				
8	Ge	4.875250	4.180465	0.000000			
9	Ge	2.582980	4.894991	3.630776	0.000000		
10	Ge	2.525207	2.568556	4.168949	3.623912	0.000000	
11	Ge	4.154339	4.870667	2.537381	2.585682	4.866732	0.000000



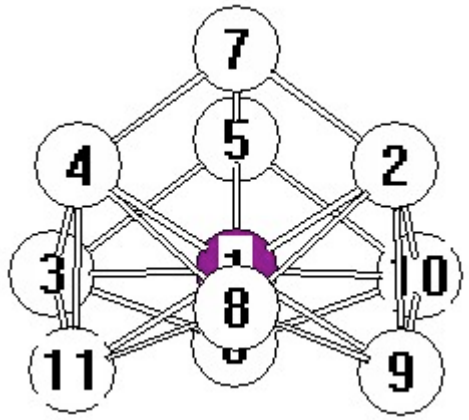
0-4 APT – C_{2v} [6] (rc-54, rb-53) → C_1 [6] [5]

- 21901.3463963 (+26.60 kcal/mol) ** i -22 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.610965	0.000000				
3	Ge	2.578945	5.043368	0.000000			
4	Ge	2.610380	3.844879	2.883484	0.000000		
5	Ge	2.610380	3.844879	2.883484	3.848512	0.000000	
6	Ge	2.561866	4.647663	2.617120	4.647127	2.507461	
7	Ge	2.692552	2.581449	3.870954	2.584045	2.584045	
8	Ge	2.579817	2.888413	4.453611	2.886495	5.046670	
9	Ge	2.563087	2.507723	4.958874	4.646376	4.646376	
10	Ge	2.579817	2.888413	4.453611	5.046670	2.886495	
11	Ge	2.561866	4.647663	2.617120	2.507461	4.647127	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.463529	0.000000				
8	Ge	4.954965	3.878240	0.000000			
9	Ge	3.981083	4.462470	2.613917	0.000000		
10	Ge	2.615176	3.878240	4.452898	2.613917	0.000000	
11	Ge	3.977754	4.463529	2.615176	3.981083	4.954965	0.000000



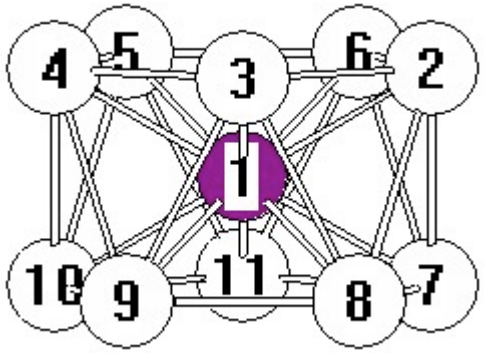
0-4 APT – C_{2v} [6] (rd-29) → C_s [6] [8]

- 21901.3256021 (+39.65 kcal/mol)

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.529656	0.000000				
3	Ge	2.529656	2.582124	0.000000			
4	Ge	2.529656	4.177964	2.582124	0.000000		
5	Ge	2.529656	4.177964	4.177964	2.582124	0.000000	
6	Ge	2.529656	2.582124	4.177964	4.177964	2.582124	
7	Ge	2.529656	2.853287	4.350778	5.059311	4.350778	
8	Ge	2.529656	2.853287	2.853287	4.350778	5.059311	
9	Ge	2.529656	4.350778	2.853287	2.853287	4.350778	
10	Ge	2.529656	5.059311	4.350778	2.853287	2.853287	
11	Ge	2.529656	4.350778	5.059311	4.350778	2.853287	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.853287	0.000000				
8	Ge	4.350778	2.582124	0.000000			
9	Ge	5.059311	4.177964	2.582124	0.000000		
10	Ge	4.350778	4.177964	4.177964	2.582124	0.000000	
11	Ge	2.853287	2.582124	4.177964	4.177964	2.582124	0.000000



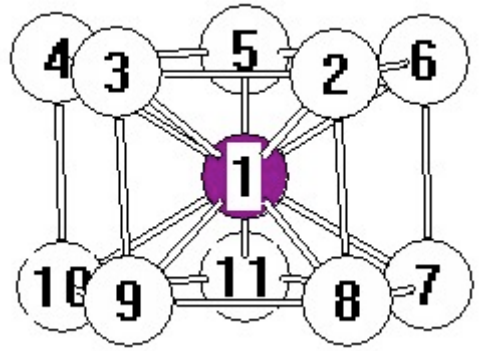
0-5 APP – D_{5d} [4] [6]

- 21901.3446862 (+27.67 kcal/mol) ** i -86 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.503150	0.000000				
3	Ge	2.574381	2.479155	0.000000			
4	Ge	2.578005	4.069521	2.484482	0.000000		
5	Ge	2.492984	4.147724	4.092637	2.561432	0.000000	
6	Ge	2.450990	2.564161	4.096959	4.155474	2.621411	
7	Ge	2.492984	3.655647	4.882783	4.929287	3.687848	
8	Ge	2.578005	2.589466	3.684309	4.923525	4.929287	
9	Ge	2.574381	3.495517	2.602960	3.684309	4.882783	
10	Ge	2.503150	4.719323	3.495517	2.589466	3.655647	
11	Ge	2.450990	4.841729	4.799198	3.612757	2.565948	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.565948	0.000000				
8	Ge	3.612757	2.561432	0.000000			
9	Ge	4.799198	4.092637	2.484482	0.000000		
10	Ge	4.841729	4.147724	4.069521	2.479155	0.000000	
11	Ge	3.647605	2.621411	4.155474	4.096959	2.564161	0.000000



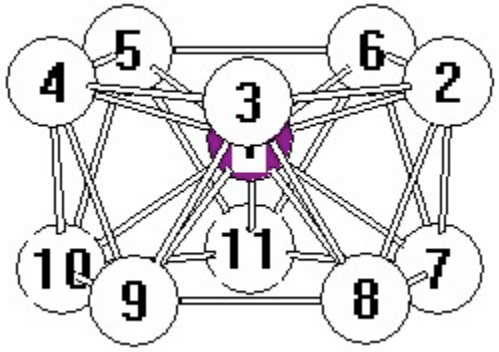
0-5 APP – D_{5d} [4] (r-86) → C_2 [4] [1]

- 21901.3887932 (**+0.00 kcal/mol**) ** i -10 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.485440	0.000000				
3	Ge	2.485954	2.790180	0.000000			
4	Ge	2.488258	4.508309	2.784302	0.000000		
5	Ge	2.488258	4.508309	4.504852	2.780028	0.000000	
6	Ge	2.485954	2.790180	4.511232	4.504852	2.784302	
7	Ge	2.751379	2.743046	4.411865	5.178949	4.411460	
8	Ge	2.751379	2.743046	2.742336	4.411460	5.178949	
9	Ge	2.751461	4.410958	2.741100	2.744264	4.405683	
10	Ge	2.757366	5.183002	4.409146	2.740809	2.740809	
11	Ge	2.751461	4.410958	5.175917	4.405683	2.744264	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.742336	0.000000				
8	Ge	4.411865	2.647647	0.000000			
9	Ge	5.175917	4.279864	2.646478	0.000000		
10	Ge	4.409146	4.286384	4.286384	2.644372	0.000000	
11	Ge	2.741100	2.646478	4.279864	4.272998	2.644372	0.000000



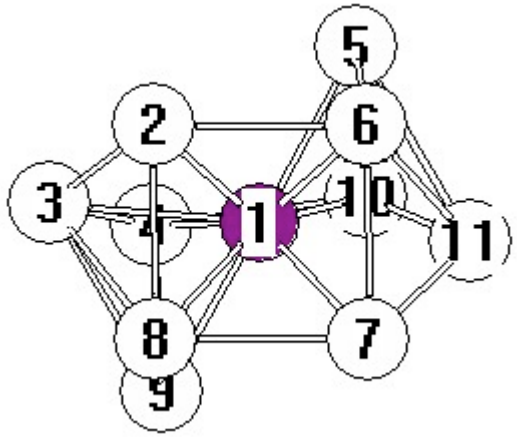
0-5 APP – D_{5d} [8] (ra-422) → C_s [8] [14]

- 21901.2661610 (+76.95 kcal/mol)

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.661311	0.000000				
3	Ge	2.643913	2.552121	0.000000			
4	Ge	2.625717	4.388618	2.597773	0.000000		
5	Ge	2.548792	3.654097	4.328899	3.811862	0.000000	
6	Ge	2.628301	2.666666	4.514250	5.105888	2.595900	
7	Ge	2.658512	3.789242	4.681905	5.051300	4.291102	
8	Ge	2.627471	2.665760	2.777988	4.257454	4.960127	
9	Ge	2.549512	4.287034	2.836942	2.573350	4.945094	
10	Ge	2.626734	5.051337	4.545019	2.694236	2.571065	
11	Ge	2.643491	4.680529	5.286787	4.545406	2.844774	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.669238	0.000000				
8	Ge	3.752957	2.665297	0.000000			
9	Ge	4.965228	3.662124	2.597736	0.000000		
10	Ge	4.251993	4.389536	5.110341	3.825332	0.000000	
11	Ge	2.772388	2.552585	4.515373	4.343929	2.598931	0.000000



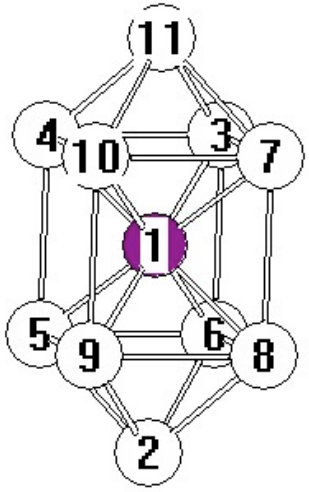
0-5 APP – D_{5d} [8] (rb-224, ra-43) → C_1 [8] [13]

- 21901.2741940 (+71.91 kcal/mol)

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.185586	0.000000				
3	Ge	2.464332	5.091196	0.000000			
4	Ge	2.464332	5.091196	2.740535	0.000000		
5	Ge	2.464332	2.553722	4.096485	3.044775	0.000000	
6	Ge	2.464332	2.553722	3.044775	4.096485	2.740535	
7	Ge	2.464332	5.091196	2.740535	3.875702	4.928664	
8	Ge	2.464332	2.553722	4.096485	4.928664	3.875702	
9	Ge	2.464332	2.553722	4.928664	4.096485	2.740535	
10	Ge	2.464332	5.091196	3.875702	2.740535	4.096485	
11	Ge	3.185586	6.371171	2.553722	2.553722	5.091196	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.096485	0.000000				
8	Ge	2.740535	3.044775	0.000000			
9	Ge	3.875702	4.096485	2.740535	0.000000		
10	Ge	4.928664	2.740535	4.096485	3.044775	0.000000	
11	Ge	5.091196	2.553722	5.091196	5.091196	2.553722	0.000000



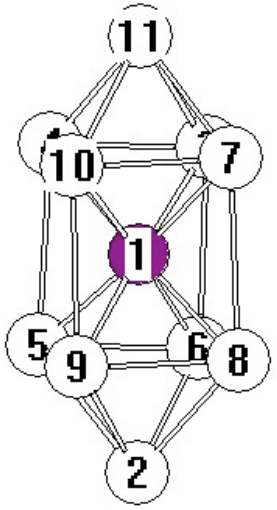
0-8 CBO – D_{4h} [2] [11]

- 21901.3012777 (+54.92 kcal/mol)

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.519529	0.000000				
3	Ge	2.501272	5.460146	0.000000			
4	Ge	2.411321	5.468533	2.606579	0.000000		
5	Ge	2.501272	2.733806	4.189122	3.254824	0.000000	
6	Ge	2.411321	2.549169	3.254824	4.142169	2.606579	
7	Ge	2.411321	5.468533	2.606579	3.492940	4.909271	
8	Ge	2.501272	2.733806	4.189122	4.909271	3.866962	
9	Ge	2.411321	2.549169	4.909271	4.142169	2.606579	
10	Ge	2.501272	5.460146	3.866962	2.606579	4.189122	
11	Ge	3.519529	7.039059	2.733806	2.549169	5.460146	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.142169	0.000000				
8	Ge	2.606579	3.254824	0.000000			
9	Ge	3.492940	4.142169	2.606579	0.000000		
10	Ge	4.909271	2.606579	4.189122	3.254824	0.000000	
11	Ge	5.468533	2.549169	5.460146	5.468533	2.733806	0.000000



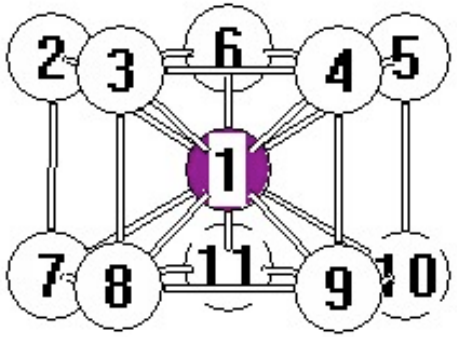
0-8 CBO – D_{4h} [6] (r-107) → D_{2d} [6] [12]

- 21901.2953792 (+58.62 kcal/mol)

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.496708	0.000000				
3	Ge	2.496708	2.532582	0.000000			
4	Ge	2.496708	4.097803	2.532582	0.000000		
5	Ge	2.496708	4.097803	4.097803	2.532582	0.000000	
6	Ge	2.496708	2.532582	4.097803	4.097803	2.532582	
7	Ge	2.496708	2.523773	3.575388	4.812631	4.812631	
8	Ge	2.496708	3.575388	2.523773	3.575388	4.812631	
9	Ge	2.496708	4.812631	3.575388	2.523773	3.575388	
10	Ge	2.496708	4.812631	4.812631	3.575388	2.523773	
11	Ge	2.496708	3.575388	4.812631	4.812631	3.575388	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.575388	0.000000				
8	Ge	4.812631	2.532582	0.000000			
9	Ge	4.812631	4.097803	2.532582	0.000000		
10	Ge	3.575388	4.097803	4.097803	2.532582	0.000000	
11	Ge	2.523773	2.532582	4.097803	4.097803	2.532582	0.000000



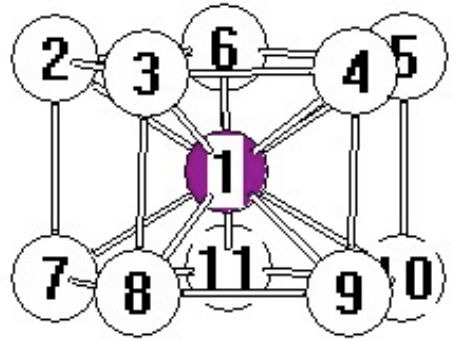
0-9 PPG – D_{5h} [4] [2]

- 21901.3861886 (+1.63 kcal/mol) ** i -40 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.458979	0.000000				
3	Ge	2.467688	2.609646	0.000000			
4	Ge	2.542773	4.124497	2.514427	0.000000		
5	Ge	2.588560	4.124058	4.077143	2.470278	0.000000	
6	Ge	2.541856	2.599158	4.163433	4.075923	2.518782	
7	Ge	2.458979	2.563888	3.647583	4.857680	4.870758	
8	Ge	2.541856	3.668906	2.575704	3.672365	4.912301	
9	Ge	2.588560	4.870758	3.543103	2.597675	3.690484	
10	Ge	2.542773	4.857680	4.739849	3.474750	2.597675	
11	Ge	2.467688	3.647583	4.834954	4.739849	3.543103	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.668906	0.000000				
8	Ge	4.953451	2.599158	0.000000			
9	Ge	4.912301	4.124058	2.518782	0.000000		
10	Ge	3.672365	4.124497	4.075923	2.470278	0.000000	
11	Ge	2.575704	2.609646	4.163433	4.077143	2.514427	0.000000



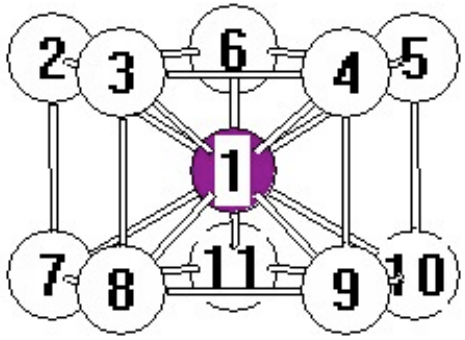
0-9 PPG – D_{5h} [4] (r-40, ra-182) → C_2 [4] [1]

- 21901.3887705 (**+0.01 kcal/mol**) ** i -10 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.567100	0.000000				
3	Ge	2.567100	2.621583	0.000000			
4	Ge	2.567100	4.241810	2.621583	0.000000		
5	Ge	2.567100	4.241810	4.241810	2.621583	0.000000	
6	Ge	2.567100	2.621583	4.241810	4.241810	2.621583	
7	Ge	2.567100	2.543126	3.652422	4.945750	4.945750	
8	Ge	2.567100	3.652422	2.543126	3.652422	4.945750	
9	Ge	2.567100	4.945750	3.652422	2.543126	3.652422	
10	Ge	2.567100	4.945750	4.945750	3.652422	2.543126	
11	Ge	2.567100	3.652422	4.945750	4.945750	3.652422	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.652422	0.000000				
8	Ge	4.945750	2.621583	0.000000			
9	Ge	4.945750	4.241810	2.621583	0.000000		
10	Ge	3.652422	4.241810	4.241810	2.621583	0.000000	
11	Ge	2.543126	2.621583	4.241810	4.241810	2.621583	0.000000



0-9 PPG – D_{5h} [8] [10]

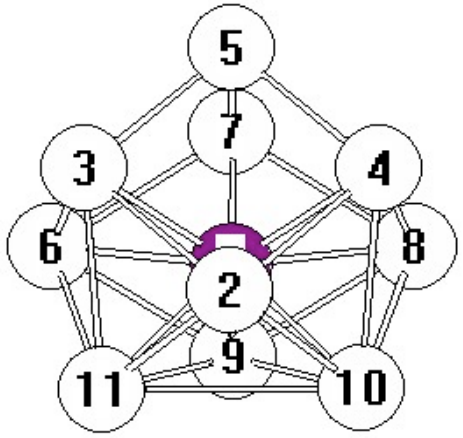
- 21901.3024415 (+54.19 kcal/mol)

$Mn@Ge_{10}^-$

Charge 1-

	1	2	3	4	5
1 Mn	0.000000				
2 Ge	2.543578	0.000000			
3 Ge	2.456905	2.674224	0.000000		
4 Ge	2.456905	2.674224	3.575949	0.000000	
5 Ge	2.659701	3.651889	2.454703	2.454703	0.000000
6 Ge	2.543578	4.405089	2.674224	4.785796	3.651889
7 Ge	2.456905	4.785796	3.575949	3.575949	2.454703
8 Ge	2.543578	4.405089	4.785796	2.674224	3.651889
9 Ge	2.292829	4.588749	4.333112	4.333112	4.449686
10 Ge	2.292829	2.688176	4.333112	2.747493	4.449686
11 Ge	2.292829	2.688176	2.747493	4.333112	4.449686

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.674224	0.000000				
8 Ge	4.405089	2.674224	0.000000			
9 Ge	2.688176	2.747493	2.688176	0.000000		
10 Ge	4.588749	4.333112	2.688176	3.139625	0.000000	
11 Ge	2.688176	4.333112	4.588749	3.139625	3.139625	0.000000



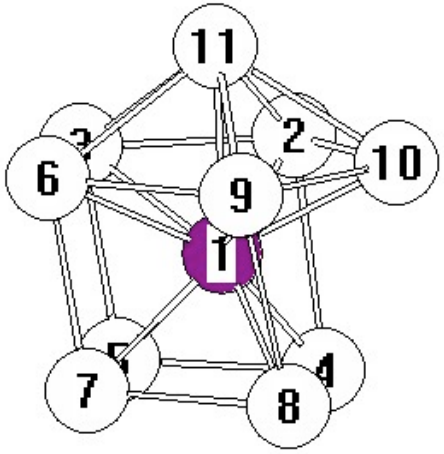
0-3 CCD – C_{3v} [1] **[6]**

- 21901.3851283 (+7.64 kcal/mol)

Charge 1-

	1	2	3	4	5
1 Mn	0.000000				
2 Ge	2.515150	0.000000			
3 Ge	2.630068	2.691303	0.000000		
4 Ge	2.428107	2.955857	4.110904	0.000000	
5 Ge	2.522016	3.536339	2.702419	2.574213	0.000000
6 Ge	2.646043	4.348022	2.679691	4.959253	3.771585
7 Ge	2.534283	4.863839	3.757542	3.739798	2.563668
8 Ge	2.437849	4.597067	4.945192	2.840694	3.714052
9 Ge	2.528882	4.383304	4.369526	4.579194	4.844288
10 Ge	2.505397	2.734470	4.407664	3.403088	4.807541
11 Ge	2.609311	2.725541	2.806389	4.657192	4.609968

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.702096	0.000000				
8 Ge	4.114130	2.566913	0.000000			
9 Ge	2.695907	3.485420	2.909238	0.000000		
10 Ge	4.398595	4.802154	3.404061	2.740330	0.000000	
11 Ge	2.766837	4.585380	4.640954	2.731099	2.677811	0.000000



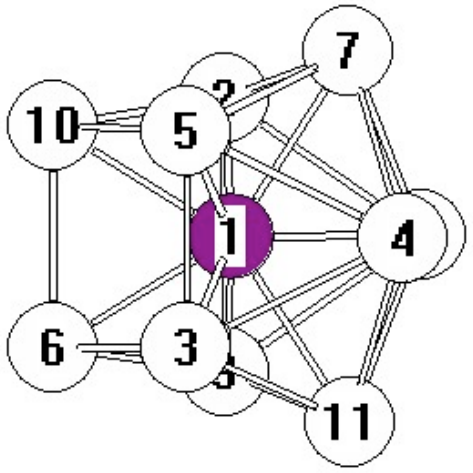
0-3 CCD – C_s [7] **(r-59) → C_1** [7] **[9]**

- 21901.3490398 (+30.29 kcal/mol) ** i -33 **

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.318581	0.000000				
3	Ge	2.463822	4.723205	0.000000			
4	Ge	2.653558	4.336101	2.792595	0.000000		
5	Ge	2.468519	3.816601	2.486624	2.788417	0.000000	
6	Ge	2.404357	3.848062	2.566523	4.567774	3.594697	
7	Ge	2.549260	2.630731	4.175855	2.588937	2.623963	
8	Ge	2.393885	2.822794	4.270208	2.801061	4.269561	
9	Ge	2.316225	3.127634	3.810878	4.336931	4.725994	
10	Ge	2.401067	2.619879	3.586825	4.558959	2.563827	
11	Ge	2.545572	4.493106	2.621331	2.589968	4.173987	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.810453	0.000000				
8	Ge	4.515985	2.696131	0.000000			
9	Ge	2.621548	4.493982	2.827160	0.000000		
10	Ge	2.538972	3.509223	4.508915	3.848446	0.000000	
11	Ge	3.517353	4.243392	2.701311	2.630510	4.805571	0.000000



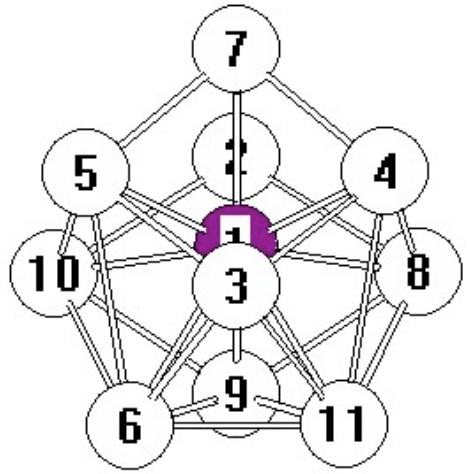
0-4 APT – C_{4v} [1] (ra-175) → C_1 [1] [5]

- 21901.3876470 (+6.06 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.308968	0.000000				
3	Ge	2.481463	4.741905	0.000000			
4	Ge	2.416818	3.845483	2.509733	0.000000		
5	Ge	2.416818	3.845483	2.509733	3.596461	0.000000	
6	Ge	2.617473	4.454605	2.700223	4.374418	3.144796	
7	Ge	2.375455	2.633104	3.589614	2.572215	2.572215	
8	Ge	2.403516	2.822562	4.022018	2.614002	4.752838	
9	Ge	2.409180	2.874799	4.262823	4.380966	4.380966	
10	Ge	2.403516	2.822562	4.022018	4.752838	2.614002	
11	Ge	2.617473	4.454605	2.700223	3.144796	4.374418	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.722933	0.000000				
8	Ge	4.274358	3.660708	0.000000			
9	Ge	2.726991	4.543061	2.718906	0.000000		
10	Ge	2.647110	3.660708	4.381103	2.718906	0.000000	
11	Ge	2.570802	4.722933	2.647110	2.726991	4.274358	0.000000



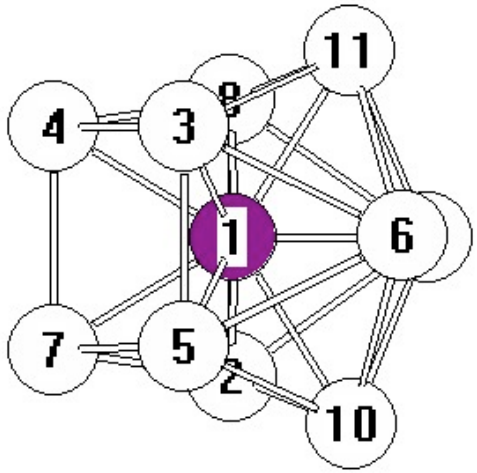
0-4 APT – C_{4v} [1] (rb-42) → C_s [1] [7]

- 21901.3847197 (+7.90 kcal/mol) ** i -83 **

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.316284	0.000000				
3	Ge	2.466009	4.725298	0.000000			
4	Ge	2.402379	3.852524	2.563593	0.000000		
5	Ge	2.465542	3.816730	2.487567	3.591147	0.000000	
6	Ge	2.651606	4.332577	2.787330	4.559128	2.792535	
7	Ge	2.401138	2.625876	3.592720	2.541520	2.566628	
8	Ge	2.318457	3.124339	3.813782	2.620958	4.725236	
9	Ge	2.394327	2.821284	4.266244	4.511040	4.269596	
10	Ge	2.548063	2.632161	4.173665	4.809167	2.620679	
11	Ge	2.550077	4.491585	2.620591	3.508168	4.177447	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.563412	0.000000				
8	Ge	4.332311	3.847568	0.000000			
9	Ge	2.795175	4.512812	2.823896	0.000000		
10	Ge	2.589825	3.513793	4.495545	2.702534	0.000000	
11	Ge	2.589131	4.808256	2.628825	2.698508	4.248151	0.000000



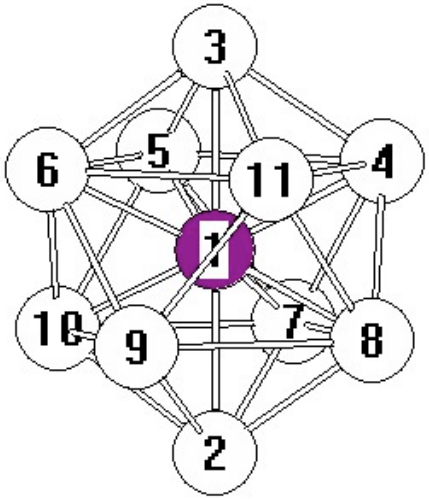
0-4 APT – C_{4v} [1] (rb-42, r-83) → C_1 [1] [5]

- 21901.3876466 (+6.06 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.530166	0.000000				
3	Ge	2.530166	5.060332	0.000000			
4	Ge	2.437600	4.205739	2.645566	0.000000		
5	Ge	2.437600	4.205739	2.645566	3.106890	0.000000	
6	Ge	2.437600	4.205739	2.645566	4.393806	3.106890	
7	Ge	2.437600	2.645566	4.205739	2.699866	2.699866	
8	Ge	2.437600	2.645566	4.205739	2.699866	4.576063	
9	Ge	2.437600	2.645566	4.205739	4.576063	4.576063	
10	Ge	2.437600	2.645566	4.205739	4.576063	2.699866	
11	Ge	2.437600	4.205739	2.645566	3.106890	4.393806	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.576063	0.000000				
8	Ge	4.576063	3.106890	0.000000			
9	Ge	2.699866	4.393806	3.106890	0.000000		
10	Ge	2.699866	3.106890	4.393806	3.106890	0.000000	
11	Ge	3.106890	4.576063	2.699866	2.699866	4.576063	0.000000



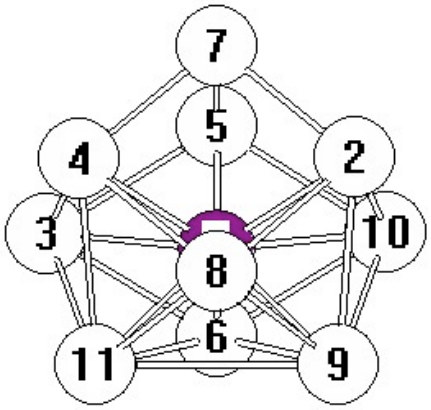
0-4 APT – D_{4d} [3] [8]

- 21901.3780128 (+12.11 kcal/mol) ** i -35 **

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.456674	0.000000				
3	Ge	2.543086	4.785527	0.000000			
4	Ge	2.455885	3.573099	2.677477	0.000000		
5	Ge	2.456565	3.575927	2.672262	3.573879	0.000000	
6	Ge	2.292141	4.330872	2.688729	4.334080	2.747924	
7	Ge	2.660494	2.454650	3.653527	2.454006	2.453540	
8	Ge	2.545488	2.670074	4.410005	2.676075	4.786304	
9	Ge	2.292508	2.747629	4.587344	4.334182	4.330581	
10	Ge	2.547174	2.675768	4.404560	4.785719	2.671124	
11	Ge	2.292322	4.329452	2.693404	2.747509	4.334734	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.449664	0.000000				
8	Ge	4.590563	3.652424	0.000000			
9	Ge	3.133430	4.450186	2.692742	0.000000		
10	Ge	2.688307	3.649004	4.409154	2.691373	0.000000	
11	Ge	3.144243	4.450133	2.687811	3.138895	4.594008	0.000000



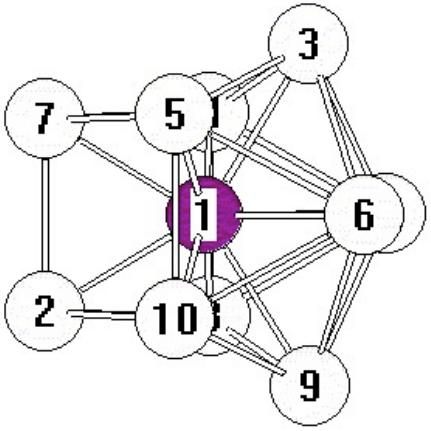
0-4 APT – D_{4d} [3] (r-35) → C_1 [1] [6]

- 21901.3851440 (+7.63 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.409007	0.000000				
3	Ge	2.590151	4.851841	0.000000			
4	Ge	2.443670	3.790645	2.697834	0.000000		
5	Ge	2.443670	3.790645	2.697834	4.105605	0.000000	
6	Ge	2.594530	4.662561	2.722627	4.348382	2.795649	
7	Ge	2.411122	2.471633	3.550870	2.805799	2.805799	
8	Ge	2.440993	2.808461	4.348671	2.635847	4.874979	
9	Ge	2.587518	3.569632	4.409643	4.345161	4.345161	
10	Ge	2.440993	2.808461	4.348671	4.874979	2.635847	
11	Ge	2.594530	4.662561	2.722627	2.795649	4.348382	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.655405	0.000000				
8	Ge	4.350490	3.797443	0.000000			
9	Ge	2.726388	4.858840	2.695711	0.000000		
10	Ge	2.803422	3.797443	4.096286	2.695711	0.000000	
11	Ge	2.701860	4.655405	2.803422	2.726388	4.350490	0.000000



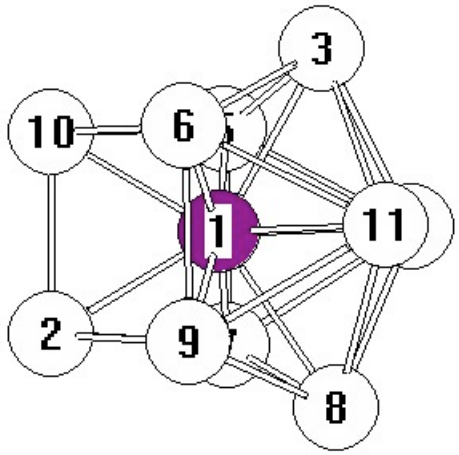
0-4 APT – C_{2v} [5] (ra-374) → C_s [5] [3]

- 21901.3924070 (+3.08 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.406885	0.000000				
3	Ge	2.578534	4.823511	0.000000			
4	Ge	2.595500	4.673714	2.721592	0.000000		
5	Ge	2.449841	3.776705	2.713152	2.769127	0.000000	
6	Ge	2.449841	3.776705	2.713152	4.352024	4.167423	
7	Ge	2.435090	2.795993	4.359273	2.825056	2.639129	
8	Ge	2.601558	3.624251	4.409074	2.726827	4.334810	
9	Ge	2.435090	2.795993	4.359273	4.345456	4.874663	
10	Ge	2.410123	2.474409	3.494917	4.640462	2.820670	
11	Ge	2.595500	4.673714	2.721592	2.704801	4.352024	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.874663	0.000000				
8	Ge	4.334810	2.678381	0.000000			
9	Ge	2.639129	4.030629	2.678381	0.000000		
10	Ge	2.820670	3.816466	4.887764	3.816466	0.000000	
11	Ge	2.769127	4.345456	2.726827	2.825056	4.640462	0.000000



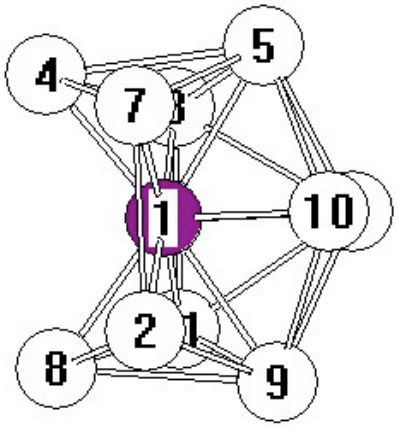
0-4 APT – C_{2v} [5] (rb-319) → C_s [5] [3]

- 21901.3923285 (+3.12 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.546706	0.000000				
3	Ge	2.555612	5.100794	0.000000			
4	Ge	2.411821	4.225401	2.565796	0.000000		
5	Ge	2.591241	4.451297	2.664679	2.881097	0.000000	
6	Ge	2.664055	4.403581	2.874231	4.431700	2.711977	
7	Ge	2.541345	2.929327	4.192228	2.564093	2.656148	
8	Ge	2.410528	2.559526	4.197312	3.815750	4.996658	
9	Ge	2.592719	2.653592	4.426261	4.999130	4.371656	
10	Ge	2.654287	2.897235	4.397323	4.447531	2.710329	
11	Ge	2.553032	4.186131	2.875613	4.180947	4.440062	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.412014	0.000000				
8	Ge	4.438105	4.198316	0.000000			
9	Ge	2.708490	4.460217	2.880315	0.000000		
10	Ge	2.628051	2.916845	4.436838	2.712637	0.000000	
11	Ge	2.894379	5.091698	2.563193	2.657861	4.402535	0.000000



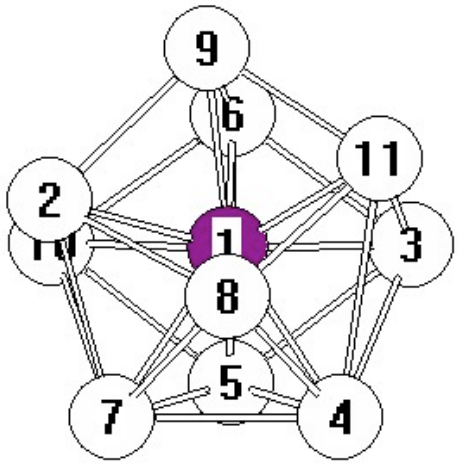
0-4 APT – C_{2v} [5] (rc-28, ra-353) → C_1 [5] [4]

- 21901.3897402 (+4.75 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.552208	0.000000				
3	Ge	2.508271	5.021969	0.000000			
4	Ge	2.506919	4.428304	2.836886	0.000000		
5	Ge	2.506919	4.428304	2.836886	2.786021	0.000000	
6	Ge	2.502769	3.997760	2.759421	4.584142	3.254040	
7	Ge	2.522049	2.865987	4.469462	2.748451	2.748451	
8	Ge	2.546909	2.722020	4.331520	2.784233	4.495847	
9	Ge	2.485965	2.722359	3.838529	4.739679	4.739679	
10	Ge	2.546909	2.722020	4.331520	4.495847	2.784233	
11	Ge	2.502769	3.997760	2.759421	3.254040	4.584142	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.583432	0.000000				
8	Ge	4.913293	2.886659	0.000000			
9	Ge	2.604892	4.612891	3.580098	0.000000		
10	Ge	2.720957	2.886659	4.472574	3.580098	0.000000	
11	Ge	3.742105	4.583432	2.720957	2.604892	4.913293	0.000000



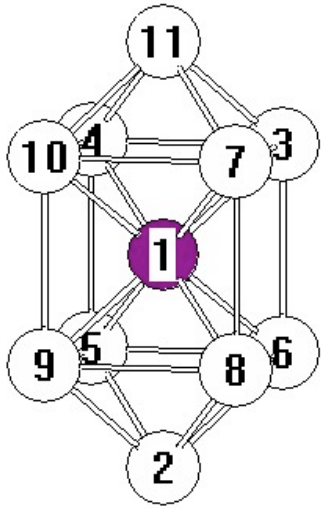
0-4 APT – C_{2v} [7] (r-50) → C_s [7] [10]

- 21901.3487344 (+30.48 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.007958	0.000000				
3	Ge	2.468754	4.900960	0.000000			
4	Ge	2.468754	4.900960	2.799096	0.000000		
5	Ge	2.468754	2.503140	4.067438	2.951121	0.000000	
6	Ge	2.468754	2.503140	2.951121	4.067438	2.799096	
7	Ge	2.468754	4.900960	2.799096	3.958519	4.937509	
8	Ge	2.468754	2.503140	4.067438	4.937509	3.958519	
9	Ge	2.468754	2.503140	4.937509	4.067438	2.799096	
10	Ge	2.468754	4.900960	3.958519	2.799096	4.067438	
11	Ge	3.007958	6.015916	2.503140	2.503140	4.900960	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.067438	0.000000				
8	Ge	2.799096	2.951121	0.000000			
9	Ge	3.958519	4.067438	2.799096	0.000000		
10	Ge	4.937509	2.799096	4.067438	2.951121	0.000000	
11	Ge	4.900960	2.503140	4.900960	4.900960	2.503140	0.000000



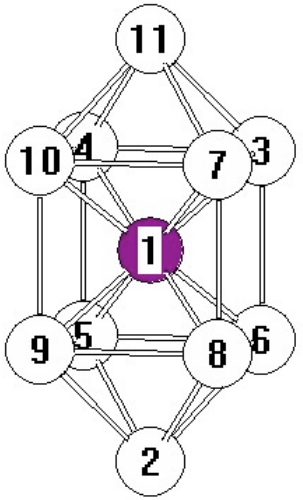
0-8 CBO – D_{4h} [1] [13]

- 21901.3210503 (+47.85 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.161154	0.000000				
3	Ge	2.396136	4.965254	0.000000			
4	Ge	2.396136	4.965254	2.739038	0.000000		
5	Ge	2.396136	2.610550	3.932371	2.821562	0.000000	
6	Ge	2.396136	2.610550	2.821562	3.932371	2.739038	
7	Ge	2.396136	4.965254	2.739038	3.873584	4.792272	
8	Ge	2.396136	2.610550	3.932371	4.792272	3.873584	
9	Ge	2.396136	2.610550	4.792272	3.932371	2.739038	
10	Ge	2.396136	4.965254	3.873584	2.739038	3.932371	
11	Ge	3.161154	6.322308	2.610550	2.610550	4.965254	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.932371	0.000000				
8	Ge	2.739038	2.821562	0.000000			
9	Ge	3.873584	3.932371	2.739038	0.000000		
10	Ge	4.792272	2.739038	3.932371	2.821562	0.000000	
11	Ge	4.965254	2.610550	4.965254	4.965254	2.610550	0.000000



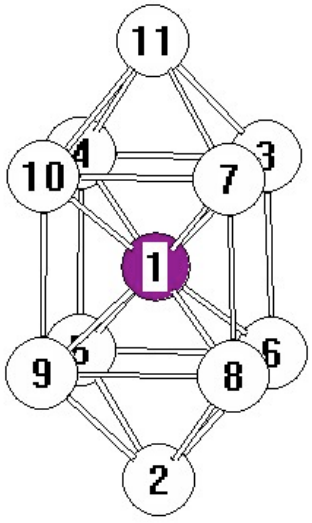
0-8 CBO – D_{4h} [5] [12]

- 21901.3470885 (+31.51 kcal/mol) ** i -30 **

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.057580	0.000000				
3	Ge	2.395803	4.899058	0.000000			
4	Ge	2.395803	4.899058	2.689207	0.000000		
5	Ge	2.399971	2.591093	3.937145	2.830972	0.000000	
6	Ge	2.399971	2.591093	2.830972	3.937145	2.783983	
7	Ge	2.395803	4.899058	2.689207	3.803114	4.794562	
8	Ge	2.399971	2.591093	3.937145	4.794562	3.937147	
9	Ge	2.399971	2.591093	4.794562	3.937145	2.783983	
10	Ge	2.395803	4.899058	3.803114	2.689207	3.937145	
11	Ge	3.271401	6.328981	2.628040	2.628040	5.044194	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.937145	0.000000				
8	Ge	2.783983	2.830972	0.000000			
9	Ge	3.937147	3.937145	2.783983	0.000000		
10	Ge	4.794562	2.689207	3.937145	2.830972	0.000000	
11	Ge	5.044194	2.628040	5.044194	5.044194	2.628040	0.000000



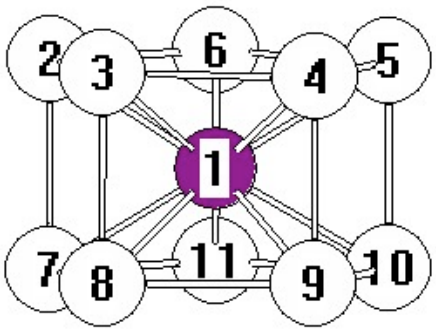
0-8 CBO – D_{4h} [5] (r-30) → C_{4v} [5] [11]

- 21901.3471242 (+31.49 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.463874	0.000000				
3	Ge	2.484952	2.447576	0.000000			
4	Ge	2.503078	4.058682	2.541137	0.000000		
5	Ge	2.503078	4.058682	4.139976	2.651286	0.000000	
6	Ge	2.484952	2.447576	4.028999	4.139976	2.541137	
7	Ge	2.463874	2.526737	3.516323	4.770611	4.770611	
8	Ge	2.484952	3.516323	2.522581	3.568314	4.838894	
9	Ge	2.503078	4.770611	3.568314	2.487725	3.635669	
10	Ge	2.503078	4.770611	4.838894	3.635669	2.487725	
11	Ge	2.484952	3.516323	4.753551	4.838894	3.568314	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.516323	0.000000				
8	Ge	4.753551	2.447576	0.000000			
9	Ge	4.838894	4.058682	2.541137	0.000000		
10	Ge	3.568314	4.058682	4.139976	2.651286	0.000000	
11	Ge	2.522581	2.447576	4.028999	4.139976	2.541137	0.000000



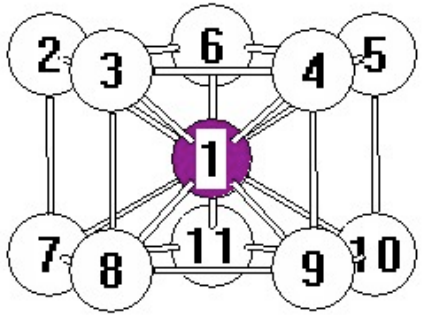
0-9 PPG – C_{2v} [1] [2]

- 21901.3932892 (+2.52 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.485710	0.000000				
3	Ge	2.485710	2.521784	0.000000			
4	Ge	2.485710	4.080332	2.521784	0.000000		
5	Ge	2.485710	4.080332	4.080332	2.521784	0.000000	
6	Ge	2.485710	2.521784	4.080332	4.080332	2.521784	
7	Ge	2.485710	2.511615	3.559158	4.791380	4.791380	
8	Ge	2.485710	3.559158	2.511615	3.559158	4.791380	
9	Ge	2.485710	4.791380	3.559158	2.511615	3.559158	
10	Ge	2.485710	4.791380	4.791380	3.559158	2.511615	
11	Ge	2.485710	3.559158	4.791380	4.791380	3.559158	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.559158	0.000000				
8	Ge	4.791380	2.521784	0.000000			
9	Ge	4.791380	4.080332	2.521784	0.000000		
10	Ge	3.559158	4.080332	4.080332	2.521784	0.000000	
11	Ge	2.511615	2.521784	4.080332	4.080332	2.521784	0.000000



0-9 PPG – D_{5h} [3] [1]

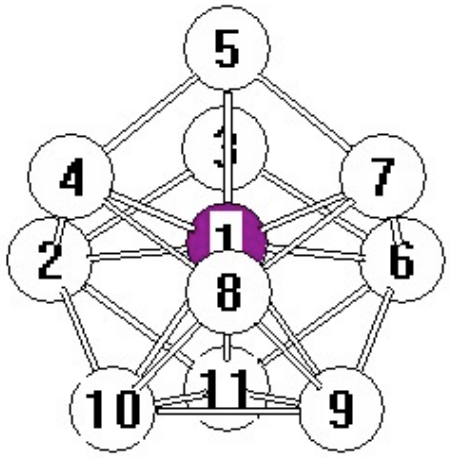
- 21901.3973085 (**+0.00 kcal/mol**)

$Mn@Ge_{10}$

Charge 0

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.498316	0.000000				
3 Ge	2.399194	2.681107	0.000000			
4 Ge	2.399194	2.681107	3.816944	0.000000		
5 Ge	2.405866	3.696708	2.641984	2.641984	0.000000	
6 Ge	2.498316	4.286957	2.681107	4.852980	3.696708	
7 Ge	2.399194	4.852980	3.816944	3.816944	2.641984	
8 Ge	2.498316	4.286957	4.852980	2.681107	3.696708	
9 Ge	2.548642	4.402184	4.421511	4.421511	4.666818	
10 Ge	2.548642	2.720920	4.421511	2.981098	4.666818	
11 Ge	2.548642	2.720920	2.981098	4.421511	4.666818	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.681107	0.000000				
8 Ge	4.286957	2.681107	0.000000			
9 Ge	2.720920	2.981098	2.720920	0.000000		
10 Ge	4.402184	4.421511	2.720920	2.793548	0.000000	
11 Ge	2.720920	4.421511	4.402184	2.793548	2.793548	0.000000



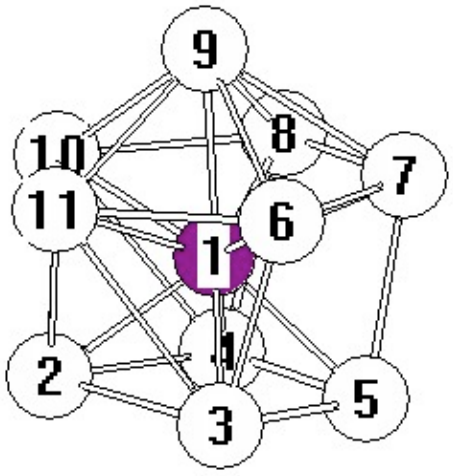
0-3 CCD – C_{3v} [4] [1]

- 21901.3042724 (**+0.01 kcal/mol**)

Charge 0

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.454522	0.000000				
3 Ge	2.486826	2.776232	0.000000			
4 Ge	2.486826	2.776232	3.774710	0.000000		
5 Ge	2.506552	3.763831	2.558820	2.558820	0.000000	
6 Ge	2.556277	4.303122	2.700859	4.913105	3.651236	
7 Ge	2.447943	4.868977	3.876785	3.876785	2.767699	
8 Ge	2.556277	4.303122	4.913105	2.700859	3.651236	
9 Ge	2.532800	4.405091	4.560920	4.560920	4.692610	
10 Ge	2.516445	2.767628	4.584909	3.225062	4.746399	
11 Ge	2.516445	2.767628	3.225062	4.584909	4.746399	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.659944	0.000000				
8 Ge	4.462318	2.659944	0.000000			
9 Ge	2.879617	2.833903	2.879617	0.000000		
10 Ge	4.516034	4.357304	2.799923	2.771743	0.000000	
11 Ge	2.799923	4.357304	4.516034	2.771743	2.813560	0.000000



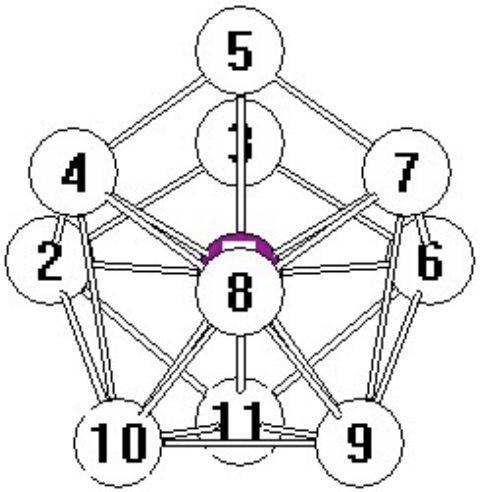
0-3 CCD – C_s [6] [6]

- 21901.2639603 (+25.30 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.551866	0.000000				
3	Ge	2.585689	2.719648	0.000000			
4	Ge	2.585689	2.719648	3.866866	0.000000		
5	Ge	2.595834	3.611320	2.579130	2.579130	0.000000	
6	Ge	2.551866	4.419412	2.719648	4.948309	3.611320	
7	Ge	2.585689	4.948309	3.866866	3.866866	2.579130	
8	Ge	2.551866	4.419412	4.948309	2.719648	3.611320	
9	Ge	2.477109	4.587815	4.618174	4.618174	4.755957	
10	Ge	2.477109	2.945253	4.618174	3.240529	4.755957	
11	Ge	2.477109	2.945253	3.240529	4.618174	4.755957	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.719648	0.000000				
8	Ge	4.419412	2.719648	0.000000			
9	Ge	2.945253	3.240529	2.945253	0.000000		
10	Ge	4.587815	4.618174	2.945253	2.799814	0.000000	
11	Ge	2.945253	4.618174	4.587815	2.799814	2.799814	0.000000



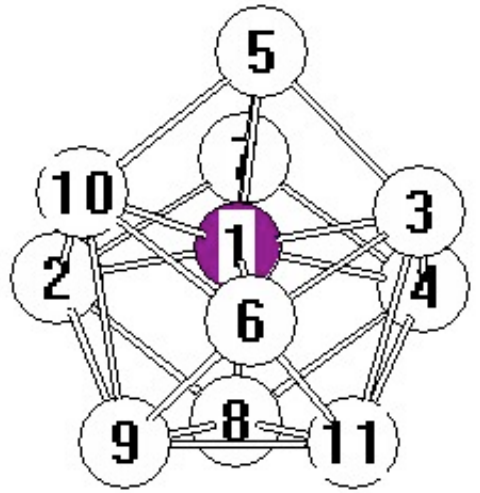
0-3 CCD – C_{3v} [8] [8]

- 21901.2275523 (+48.15 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.402937	0.000000				
3	Ge	2.400962	4.803854	0.000000			
4	Ge	2.527025	4.194023	2.599497	0.000000		
5	Ge	2.268910	3.811202	2.687551	3.677062	0.000000	
6	Ge	2.527505	4.195357	2.599739	4.181471	3.676038	
7	Ge	2.324259	2.719988	3.859933	2.622637	2.784645	
8	Ge	2.673663	2.682421	4.326155	2.682289	4.749403	
9	Ge	2.673753	2.683054	4.326438	4.297848	4.748697	
10	Ge	2.324386	2.720342	3.860778	4.841724	2.785022	
11	Ge	2.652080	4.197712	2.844610	2.634233	4.604050	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.841946	0.000000				
8	Ge	4.297916	3.002277	0.000000			
9	Ge	2.682719	4.437861	2.696650	0.000000		
10	Ge	2.622303	3.961769	4.436810	2.999870	0.000000	
11	Ge	2.633949	4.309558	2.618184	2.618368	4.308366	0.000000



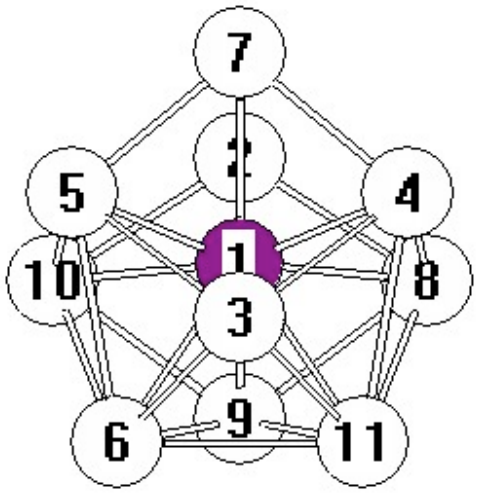
0-4 APT – C_{4v} [2] (r-54) → C_1 [2] [2]

- 21901.3012639 (+1.90 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.397673	0.000000				
3	Ge	2.502544	4.852969	0.000000			
4	Ge	2.398614	3.810129	2.683426	0.000000		
5	Ge	2.398614	3.810129	2.683426	3.826873	0.000000	
6	Ge	2.549440	4.429037	2.720093	4.418194	2.970997	
7	Ge	2.407055	2.638384	3.690559	2.644402	2.644402	
8	Ge	2.497624	2.680557	4.293215	2.677410	4.852763	
9	Ge	2.546426	2.996473	4.402799	4.414194	4.414194	
10	Ge	2.497624	2.680557	4.293215	4.852763	2.677410	
11	Ge	2.549440	4.429037	2.720093	2.970997	4.418194	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.665168	0.000000				
8	Ge	4.404739	3.700619	0.000000			
9	Ge	2.794714	4.671849	2.718620	0.000000		
10	Ge	2.727751	3.700619	4.280463	2.718620	0.000000	
11	Ge	2.794348	4.665168	2.727751	2.794714	4.404739	0.000000



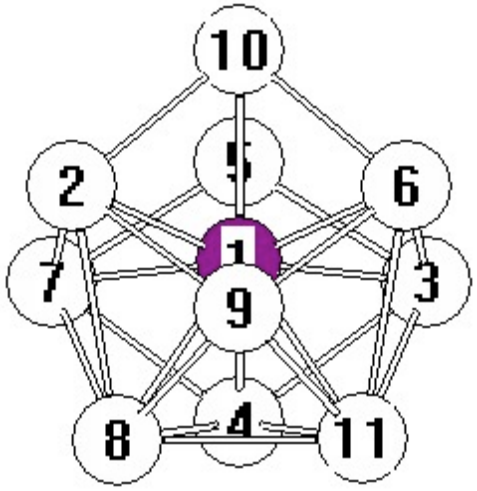
0-4 APT – C_{2v} [4] (ra-539) → C_s [4] [1]

- 21901.3042679 (**+0.01 kcal/mol**)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.397572	0.000000				
3	Ge	2.498814	4.851984	0.000000			
4	Ge	2.548047	4.419207	2.720618	0.000000		
5	Ge	2.396556	3.812650	2.682288	2.976614	0.000000	
6	Ge	2.396556	3.812650	2.682288	4.419476	3.817085	
7	Ge	2.500741	2.679490	4.290688	2.722736	2.679345	
8	Ge	2.549418	2.979231	4.403754	2.795355	4.418379	
9	Ge	2.500741	2.679490	4.290688	4.405016	4.852871	
10	Ge	2.407165	2.642850	3.697795	4.666803	2.642288	
11	Ge	2.548047	4.419207	2.720618	2.795729	4.419476	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.852871	0.000000				
8	Ge	4.418379	2.721667	0.000000			
9	Ge	2.679345	4.288997	2.721667	0.000000		
10	Ge	2.642288	3.699207	4.668596	3.699207	0.000000	
11	Ge	2.976614	4.405016	2.795355	2.722736	4.666803	0.000000



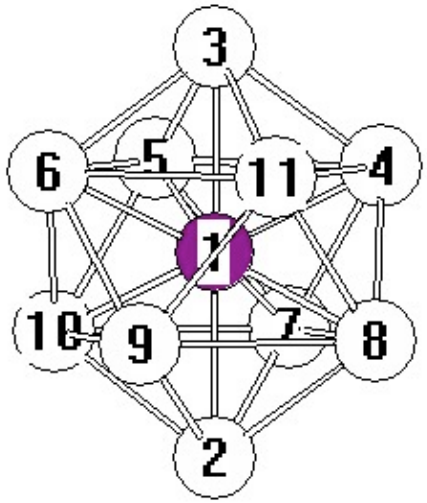
0-4 APT – C_{2v} [4] (rb-432) → C_s [4] [1]

- 21901.3042847 (**+0.00 kcal/mol**)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.624447	0.000000				
3	Ge	2.624447	5.248894	0.000000			
4	Ge	2.492289	4.323953	2.738955	0.000000		
5	Ge	2.492289	4.323953	2.738955	3.185694	0.000000	
6	Ge	2.492289	4.323953	2.738955	4.505252	3.185694	
7	Ge	2.492289	2.738955	4.323953	2.742478	2.742478	
8	Ge	2.492289	2.738955	4.323953	2.742478	4.676916	
9	Ge	2.492289	2.738955	4.323953	4.676916	4.676916	
10	Ge	2.492289	2.738955	4.323953	4.676916	2.742478	
11	Ge	2.492289	4.323953	2.738955	3.185694	4.505252	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.676916	0.000000				
8	Ge	4.676916	3.185694	0.000000			
9	Ge	2.742478	4.505252	3.185694	0.000000		
10	Ge	2.742478	3.185694	4.505252	3.185694	0.000000	
11	Ge	3.185694	4.676916	2.742478	2.742478	4.676916	0.000000



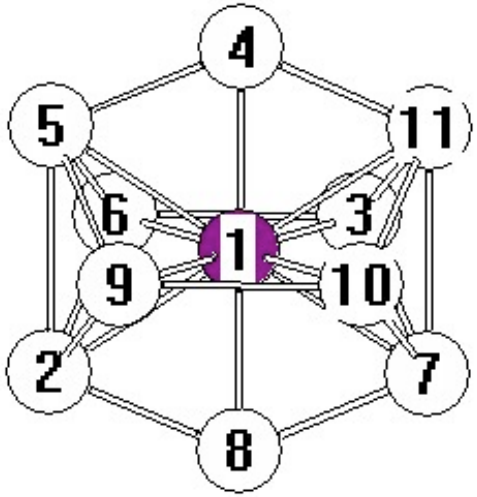
0-4 APT – D_{4d} [6] [5]

- 21901.2674897 (+23.09 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.745484	0.000000				
3	Ge	2.438225	4.486562	0.000000			
4	Ge	2.495325	4.627889	3.490672	0.000000		
5	Ge	2.745767	3.054731	4.491311	2.484729	0.000000	
6	Ge	2.441056	2.601851	2.934270	3.494740	2.603863	
7	Ge	2.751457	4.575306	2.606222	4.620527	5.497207	
8	Ge	2.494712	2.485921	3.480044	4.990013	4.628458	
9	Ge	2.441056	2.601851	4.879256	3.494740	2.603863	
10	Ge	2.438225	4.486562	3.903913	3.490672	4.491311	
11	Ge	2.742035	5.487481	2.606227	2.487197	4.571555	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.503659	0.000000				
8	Ge	3.492782	2.484717	0.000000			
9	Ge	3.892813	4.503659	3.492782	0.000000		
10	Ge	4.879256	2.606222	3.480044	2.934270	0.000000	
11	Ge	4.497651	3.027959	4.607580	4.497651	2.606227	0.000000



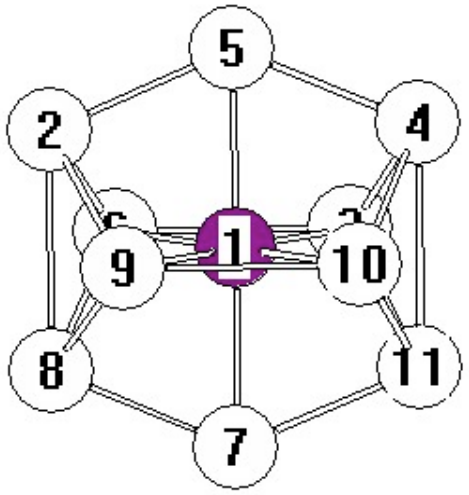
0-8 CBO – D_{4h} [4] (r-61, ra-49) → C_s [4] [7]

- 21901.2534179 (+31.92 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.752608	0.000000				
3	Ge	2.445900	4.513078	0.000000			
4	Ge	2.735810	4.568882	2.600476	0.000000		
5	Ge	2.498118	2.486329	3.504912	2.483315	0.000000	
6	Ge	2.433067	2.610715	2.927976	4.468227	3.476374	
7	Ge	2.497660	4.607330	3.507389	4.636602	4.995546	
8	Ge	2.751338	3.009044	4.513808	5.486933	4.605215	
9	Ge	2.433067	2.610715	4.878889	4.468227	3.476374	
10	Ge	2.445900	4.513078	3.896376	2.600476	3.504912	
11	Ge	2.734395	5.486857	2.600262	3.064196	4.633351	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.477612	0.000000				
8	Ge	2.610305	2.487976	0.000000			
9	Ge	3.908892	3.477612	2.610305	0.000000		
10	Ge	4.878889	3.507389	4.513808	2.927976	0.000000	
11	Ge	4.468704	2.486866	4.571296	4.468704	2.600262	0.000000



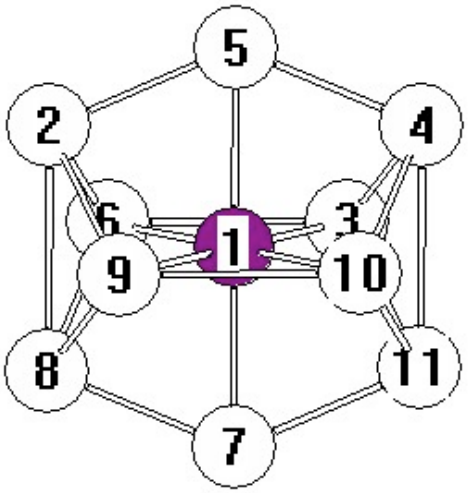
0-8 CBO – D_{4h} [4] (r-61, rb-16) → C_s [4] [7]

- 21901.2534056 (+31.93 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.736592	0.000000				
3	Ge	2.438682	4.481533	0.000000			
4	Ge	2.753839	4.572254	2.603851	0.000000		
5	Ge	2.495686	2.487855	3.483005	2.483541	0.000000	
6	Ge	2.439926	2.603772	2.929973	4.502063	3.500475	
7	Ge	2.497033	4.623511	3.482982	4.620072	4.992647	
8	Ge	2.748287	3.058592	4.487228	5.502041	4.638959	
9	Ge	2.440360	2.602064	4.879003	4.515180	3.505265	
10	Ge	2.439306	4.484246	3.899632	2.608514	3.480578	
11	Ge	2.746658	5.483218	2.604729	3.029527	4.609748	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.489518	0.000000				
8	Ge	2.602334	2.483236	0.000000			
9	Ge	3.892720	3.490493	2.603114	0.000000		
10	Ge	4.879232	3.491365	4.498350	2.943940	0.000000	
11	Ge	4.495703	2.485226	4.571723	4.498046	2.602616	0.000000



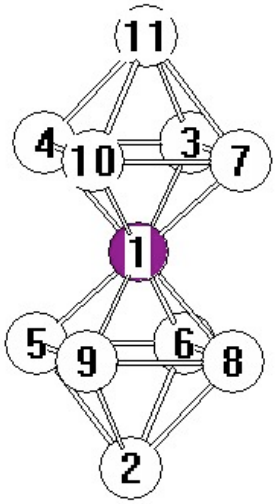
0-8 CBO – D_{4h} [4] (r-61, rc-14, r-39) → C_1 [4] [7]

- 21901.2534118 (+31.92 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.588780	0.000000				
3	Ge	2.454321	5.553205	0.000000			
4	Ge	2.454321	5.553205	2.552917	0.000000		
5	Ge	2.454321	2.639693	4.192539	3.325658	0.000000	
6	Ge	2.454321	2.639693	3.325658	4.192539	2.552917	
7	Ge	2.454321	5.553205	2.552917	3.610369	4.908642	
8	Ge	2.454321	2.639693	4.192539	4.908642	3.610369	
9	Ge	2.454321	2.639693	4.908642	4.192539	2.552917	
10	Ge	2.454321	5.553205	3.610369	2.552917	4.192539	
11	Ge	3.588780	7.177560	2.639693	2.639693	5.553205	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.192539	0.000000				
8	Ge	2.552917	3.325658	0.000000			
9	Ge	3.610369	4.192539	2.552917	0.000000		
10	Ge	4.908642	2.552917	4.192539	3.325658	0.000000	
11	Ge	5.553205	2.639693	5.553205	5.553205	2.639693	0.000000



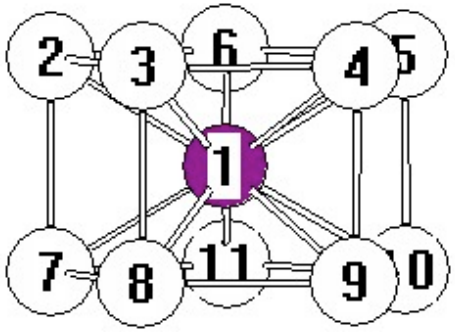
0-8 CBO – D_{4h} [8] **[9]**

- 21901.2012327 (+64.67 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.433332	0.000000				
3	Ge	2.485869	2.635186	0.000000			
4	Ge	2.557081	4.134906	2.502717	0.000000		
5	Ge	2.545949	4.115812	4.048439	2.443585	0.000000	
6	Ge	2.497474	2.632546	4.191630	4.076966	2.502589	
7	Ge	2.433323	2.496890	3.630668	4.833483	4.823326	
8	Ge	2.497402	3.635658	2.508116	3.555661	4.780540	
9	Ge	2.545762	4.823436	3.540404	2.521667	3.512258	
10	Ge	2.557327	4.833434	4.775856	3.510420	2.521795	
11	Ge	2.486091	3.630491	4.875174	4.775584	3.540205	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.635548	0.000000				
8	Ge	4.894183	2.632626	0.000000			
9	Ge	4.780204	4.115628	2.502922	0.000000		
10	Ge	3.555425	4.134457	4.077205	2.443510	0.000000	
11	Ge	2.508199	2.634791	4.191580	4.047991	2.502220	0.000000



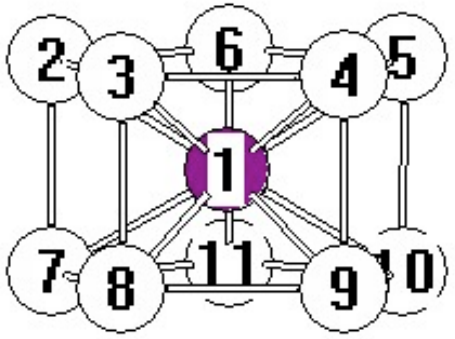
0-9 PPG – D_{5h} [2] **(ra-300, ra-157) → C_1** [2] **[3]**

- 21901.2974602 (+4.28 kcal/mol) ** i -38 **

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.484549	0.000000				
3	Ge	2.481190	2.581247	0.000000			
4	Ge	2.478313	4.121940	2.559014	0.000000		
5	Ge	2.474022	4.070884	4.087968	2.492182	0.000000	
6	Ge	2.467928	2.515950	4.093613	4.042763	2.471572	
7	Ge	2.480135	2.470536	3.568197	4.802078	4.757039	
8	Ge	2.482396	3.569832	2.463658	3.557577	4.775658	
9	Ge	2.484345	4.810490	3.555515	2.475293	3.516689	
10	Ge	2.464229	4.752188	4.765867	3.512727	2.482840	
11	Ge	2.478844	3.531674	4.790899	4.753354	3.506483	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.527795	0.000000				
8	Ge	4.782731	2.576789	0.000000			
9	Ge	4.748891	4.120663	2.559888	0.000000		
10	Ge	3.498731	4.046397	4.071301	2.490826	0.000000	
11	Ge	2.481908	2.514973	4.103726	4.063983	2.470624	0.000000



0-9 PPG – D_{5h} [2] (ra-300, ra-157, r-38) → C_1 [2] [4]

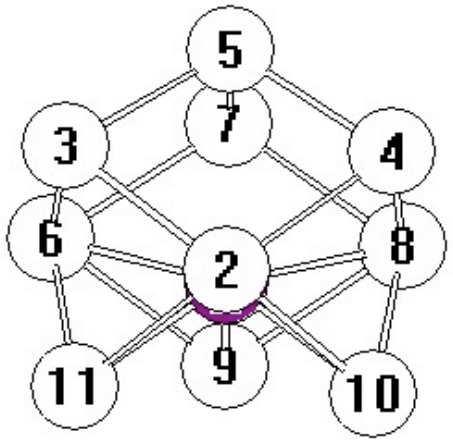
- 21901.2812036 (+14.48 kcal/mol)

$Mn@Ge_{10}^{+}$

Charge 1+

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.410749	0.000000				
3 Ge	2.763756	2.638681	0.000000			
4 Ge	2.763756	2.638681	3.810973	0.000000		
5 Ge	2.748158	3.363802	2.449135	2.449135	0.000000	
6 Ge	2.410749	4.125316	2.638681	4.762783	3.363802	
7 Ge	2.763756	4.762783	3.810973	3.810973	2.449135	
8 Ge	2.410749	4.125316	4.762783	2.638681	3.363802	
9 Ge	2.337456	4.665646	4.635421	4.635421	4.415608	
10 Ge	2.337456	2.710680	4.635421	2.857530	4.415608	
11 Ge	2.337456	2.710680	2.857530	4.635421	4.415608	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.638681	0.000000				
8 Ge	4.125316	2.638681	0.000000			
9 Ge	2.710680	2.857530	2.710680	0.000000		
10 Ge	4.665646	4.635421	2.710680	3.495602	0.000000	
11 Ge	2.710680	4.635421	4.665646	3.495602	3.495602	0.000000



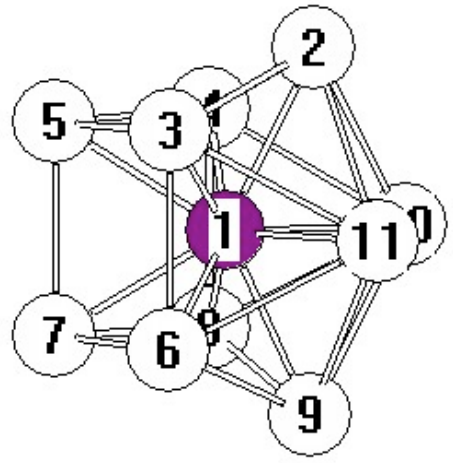
0-3 CCD – C_{3v} [3] **[7]**

- 21901.0274391 (+9.01 kcal/mol)

Charge 1+

	1	2	3	4	5	
1 Mn	0.000000					
2 Ge	2.512149	0.000000				
3 Ge	2.486714	2.705609	0.000000			
4 Ge	2.486714	2.705609	4.051354	0.000000		
5 Ge	2.508673	3.361549	2.627353	2.627353	0.000000	
6 Ge	2.490660	4.430234	2.713739	4.890169	3.749966	
7 Ge	2.501073	4.812784	3.750755	3.750755	2.633479	
8 Ge	2.490660	4.430234	4.890169	2.713739	3.749966	
9 Ge	2.509289	4.541577	4.436022	4.436022	4.804356	
10 Ge	2.512650	2.860657	4.500968	2.935355	4.630422	
11 Ge	2.512650	2.860657	2.935355	4.500968	4.630422	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.633374	0.000000				
8 Ge	4.084900	2.633374	0.000000			
9 Ge	2.708666	3.320556	2.708666	0.000000		
10 Ge	4.502118	4.615601	2.920661	2.866993	0.000000	
11 Ge	2.920661	4.615601	4.502118	2.866993	2.873707	0.000000



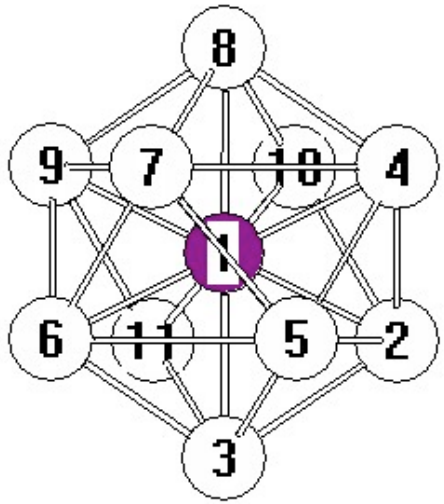
0-3 CCD – C_s [5] **[5]**

- 21901.0348084 (+4.39 kcal/mol) ** i -54 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.511846	0.000000				
3	Ge	2.496855	2.697318	0.000000			
4	Ge	2.513275	2.736579	4.219028	0.000000		
5	Ge	2.512367	3.220599	2.695542	2.734318	0.000000	
6	Ge	2.513947	4.559665	2.695693	4.714000	3.227147	
7	Ge	2.513360	4.714208	4.218407	3.232380	2.742835	
8	Ge	2.495859	4.218669	4.992697	2.693064	4.214486	
9	Ge	2.512754	4.714003	4.225516	4.559866	4.712637	
10	Ge	2.512682	2.746161	4.224200	3.231299	4.713974	
11	Ge	2.513200	3.225002	2.700548	4.713360	4.561060	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.734882	0.000000				
8	Ge	4.223980	2.696185	0.000000			
9	Ge	2.742930	3.216818	2.698983	0.000000		
10	Ge	4.711434	4.561388	2.698997	3.218936	0.000000	
11	Ge	3.225909	4.711246	4.225923	2.745480	2.735804	0.000000



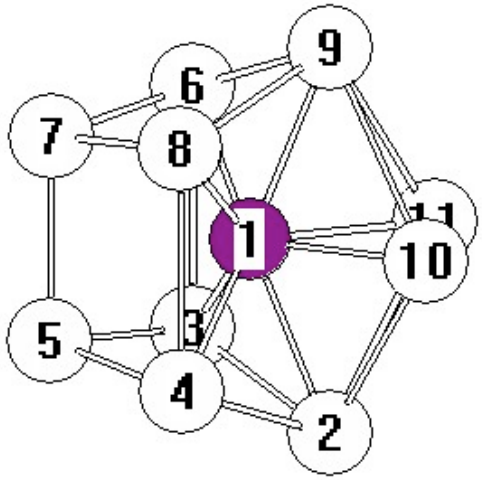
0-3 CCD – C_s [5] (r-54) → C_1 [5] [2]

- 21901.0380019 (+2.38 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.556436	0.000000				
3	Ge	2.555178	2.724516	0.000000			
4	Ge	2.551580	2.740708	3.860405	0.000000		
5	Ge	2.716878	3.535173	2.541189	2.541320	0.000000	
6	Ge	2.553181	4.638386	2.971674	4.868785	3.736018	
7	Ge	2.715780	4.943423	3.727845	3.732962	2.515425	
8	Ge	2.556993	4.656305	4.871543	2.973875	3.731713	
9	Ge	2.556432	4.749631	4.650927	4.635375	4.944796	
10	Ge	2.519226	2.987155	4.611708	3.354998	4.918631	
11	Ge	2.519887	2.940608	3.340597	4.593898	4.908327	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.539110	0.000000				
8	Ge	3.854840	2.537983	0.000000			
9	Ge	2.737606	3.535128	2.721694	0.000000		
10	Ge	4.593456	4.908721	3.347928	2.941615	0.000000	
11	Ge	3.356055	4.917611	4.615126	2.989426	2.585074	0.000000



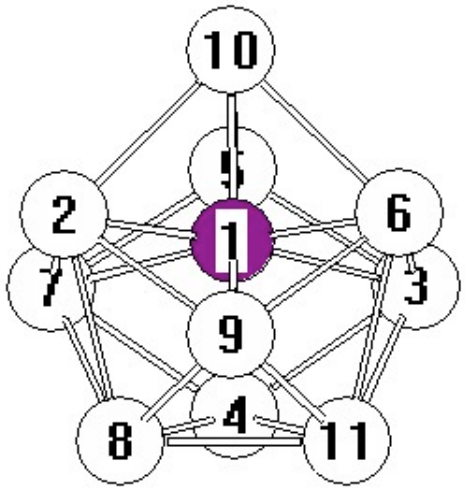
0-3 CCD – C_{3v} [9] (r-98) → C_1 [9] [22]

- 21900.9590710 (+51.91 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.314580	0.000000				
3	Ge	2.543834	4.854303	0.000000			
4	Ge	2.713920	4.279808	2.639296	0.000000		
5	Ge	2.291135	3.902974	2.665038	2.859205	0.000000	
6	Ge	2.306936	3.884810	2.662939	4.288394	3.911795	
7	Ge	2.557042	2.654551	4.253632	2.641690	2.658220	
8	Ge	2.705027	2.814191	4.238764	2.624318	4.273261	
9	Ge	2.589982	2.643682	4.262955	4.275447	4.878799	
10	Ge	2.247387	2.819922	3.886388	4.780301	2.909336	
11	Ge	2.708305	4.256042	2.631040	2.634081	4.285766	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.860309	0.000000				
8	Ge	4.251772	2.629723	0.000000			
9	Ge	2.646839	4.263228	2.628111	0.000000		
10	Ge	2.839255	3.868120	4.711890	3.811762	0.000000	
11	Ge	2.824269	4.253576	2.612154	2.633451	4.728844	0.000000



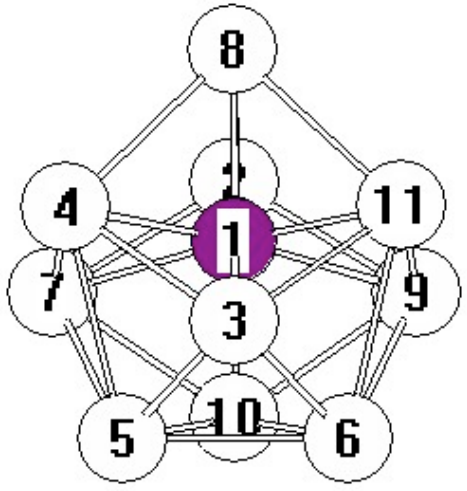
0-4 APT – D_{4d} [1] (ra-104) → C_1 [1] [1]

- 21901.0417989 (**+0.00 kcal/mol**)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.327586	0.000000				
3	Ge	2.522929	4.845507	0.000000			
4	Ge	2.298132	3.890625	2.671461	0.000000		
5	Ge	2.715606	4.262804	2.638098	2.847439	0.000000	
6	Ge	2.713650	4.266997	2.636579	4.300615	2.642636	
7	Ge	2.584718	2.641198	4.253663	2.644199	2.639578	
8	Ge	2.246698	2.789473	3.912045	2.882548	4.762064	
9	Ge	2.575647	2.644995	4.249754	4.870392	4.267936	
10	Ge	2.702755	2.794985	4.222701	4.250202	2.611337	
11	Ge	2.291506	3.892222	2.673184	3.923694	4.306304	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.272284	0.000000				
8	Ge	4.774249	3.812039	0.000000			
9	Ge	2.639604	4.263321	3.831431	0.000000		
10	Ge	2.615789	2.623023	4.684259	2.625493	0.000000	
11	Ge	2.862525	4.873654	2.896176	2.650615	4.260942	0.000000



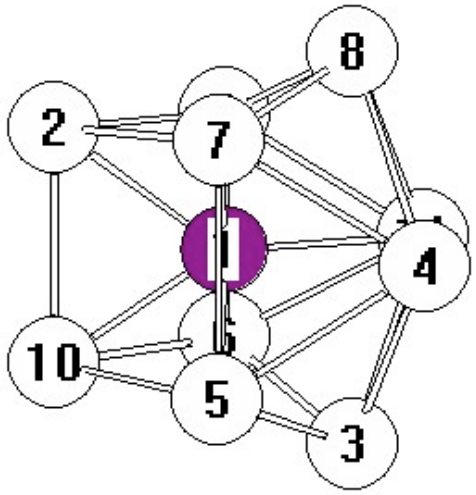
0-4 APT – D_{4d} [1] (rb-43) → C_1 [1] [1]

- 21901.0417919 (**+0.00 kcal/mol**)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.364582	0.000000				
3	Ge	2.664201	4.896876	0.000000			
4	Ge	2.637633	4.722907	2.840089	0.000000		
5	Ge	2.348852	4.037292	2.635835	2.789072	0.000000	
6	Ge	2.562016	3.703215	2.662859	4.424502	4.053894	
7	Ge	2.348435	2.908506	4.481839	2.787992	2.947996	
8	Ge	2.663804	3.479711	4.459055	2.841724	4.483127	
9	Ge	2.561240	2.628484	4.298416	4.425431	4.894435	
10	Ge	2.364642	2.663809	3.477739	4.721879	2.906715	
11	Ge	2.581854	4.440030	2.607566	2.660424	4.148311	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.894943	0.000000				
8	Ge	4.297642	2.635742	0.000000			
9	Ge	2.552650	4.053580	2.662797	0.000000		
10	Ge	2.628226	4.039115	4.896916	3.701654	0.000000	
11	Ge	2.732771	4.147355	2.607346	2.734208	4.438629	0.000000



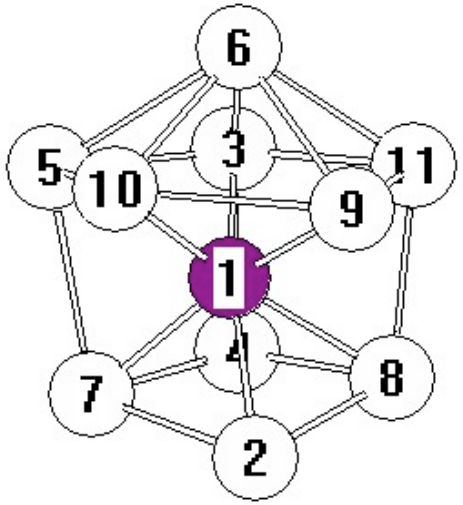
0-4 APT – C_{2v} [3] (ra-351, r-186) → C_1 [3] [6]

- 21901.0337040 (+5.08 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.335758	0.000000				
3	Ge	2.602786	4.745640	0.000000			
4	Ge	2.774580	3.751438	2.467250	0.000000		
5	Ge	2.688196	4.610462	2.515216	3.583543	0.000000	
6	Ge	2.766605	4.942266	2.624403	4.616806	2.907229	
7	Ge	2.344218	2.767239	3.585229	2.505680	2.753311	
8	Ge	2.444507	2.612133	3.518607	2.538607	4.797695	
9	Ge	2.413509	3.298149	4.149471	4.889994	4.496820	
10	Ge	2.342531	3.677218	3.962727	4.851316	2.606171	
11	Ge	2.667757	4.275283	2.577039	3.632192	4.355132	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.640991	0.000000				
8	Ge	4.491590	3.594250	0.000000			
9	Ge	2.788818	4.647603	3.377979	0.000000		
10	Ge	2.621831	3.494214	4.709586	2.835848	0.000000	
11	Ge	2.669675	4.732379	2.569528	2.594175	4.231411	0.000000



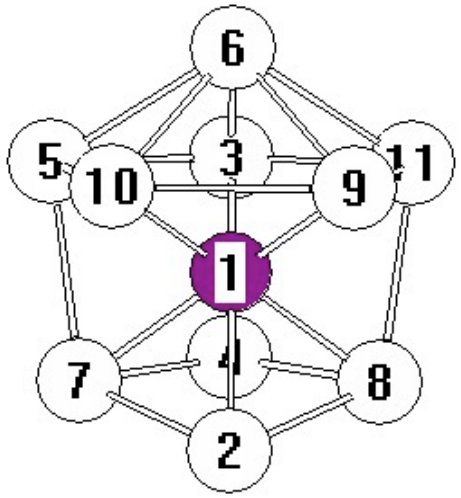
0-4 APT – C_{2v} [3] (rb-62, ra-60) → C_1 [3] [3]

- 21901.0366204 (+3.25 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.323548	0.000000				
3	Ge	2.608775	4.706397	0.000000			
4	Ge	2.800068	3.674847	2.459597	0.000000		
5	Ge	2.711770	4.480382	2.524673	3.625337	0.000000	
6	Ge	2.731353	4.940357	2.647890	4.622127	2.776065	
7	Ge	2.389056	2.647766	3.520213	2.531927	2.663888	
8	Ge	2.386477	2.650854	3.526028	2.531342	4.777616	
9	Ge	2.368038	3.561121	4.044359	4.862781	4.406875	
10	Ge	2.369651	3.552409	4.047858	4.866957	2.595622	
11	Ge	2.714303	4.491441	2.523525	3.619071	4.351701	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.522167	0.000000				
8	Ge	4.523411	3.611778	0.000000			
9	Ge	2.674609	4.685356	3.373370	0.000000		
10	Ge	2.678769	3.376979	4.682397	2.920165	0.000000	
11	Ge	2.778892	4.778021	2.669133	2.597615	4.413576	0.000000



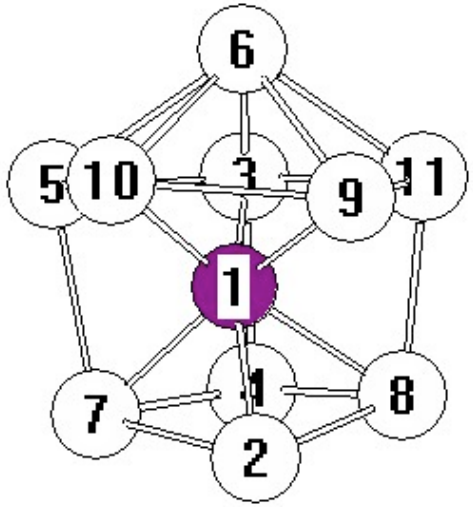
0-4 APT – C_{2v} [3] (rb-62, rb-45) → C_1 [3] [4]

- 21901.0362215 (+3.50 kcal/mol) ** i -36 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.336302	0.000000				
3	Ge	2.601813	4.748611	0.000000			
4	Ge	2.770290	3.753393	2.468968	0.000000		
5	Ge	2.686352	4.607308	2.515846	3.583266	0.000000	
6	Ge	2.765283	4.937544	2.626938	4.617000	2.914145	
7	Ge	2.343745	2.772330	3.583881	2.505370	2.746649	
8	Ge	2.443319	2.612407	3.524931	2.540036	4.798889	
9	Ge	2.414336	3.285153	4.156946	4.887626	4.500639	
10	Ge	2.342121	3.669998	3.962177	4.848717	2.606023	
11	Ge	2.665082	4.273531	2.580180	3.630588	4.356131	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.640659	0.000000				
8	Ge	4.489904	3.597126	0.000000			
9	Ge	2.793384	4.645239	3.371963	0.000000		
10	Ge	2.621705	3.491762	4.706068	2.834660	0.000000	
11	Ge	2.665674	4.731451	2.569911	2.598055	4.228026	0.000000



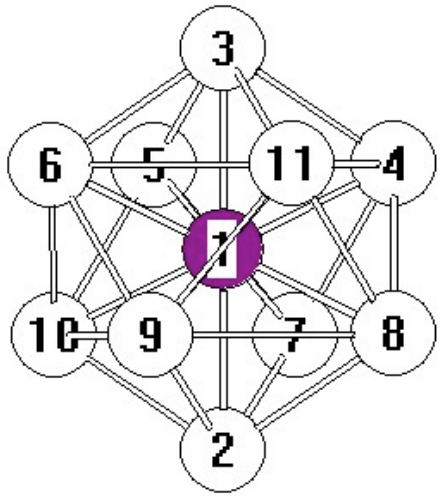
0-4 APT – C_{2v} [3] (rb-62, rb-45, r-36) → C_1 [3] [3]

- 21901.0366170 (+3.25 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.495875	0.000000				
3	Ge	2.495875	4.991749	0.000000			
4	Ge	2.513272	4.220950	2.697302	0.000000		
5	Ge	2.513272	4.220950	2.697302	3.225442	0.000000	
6	Ge	2.513272	4.220950	2.697302	4.561465	3.225442	
7	Ge	2.513272	2.697302	4.220950	2.739764	2.739764	
8	Ge	2.513272	2.697302	4.220950	2.739764	4.713708	
9	Ge	2.513272	2.697302	4.220950	4.713708	4.713708	
10	Ge	2.513272	2.697302	4.220950	4.713708	2.739764	
11	Ge	2.513272	4.220950	2.697302	3.225442	4.561465	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.713708	0.000000				
8	Ge	4.713708	3.225442	0.000000			
9	Ge	2.739764	4.561465	3.225442	0.000000		
10	Ge	2.739764	3.225442	4.561465	3.225442	0.000000	
11	Ge	3.225442	4.713708	2.739764	2.739764	4.713708	0.000000



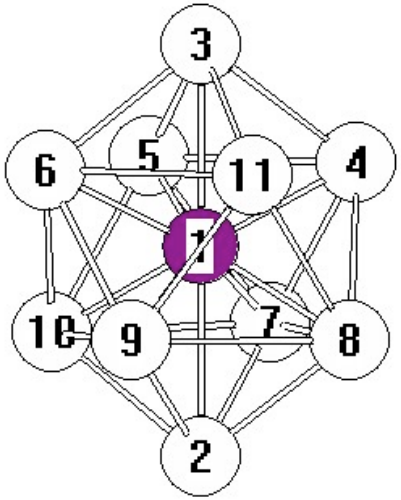
0-4 APT – D_{4d} [5] **[2]**

- 21901.0379686 (+2.40 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.769188	0.000000				
3	Ge	2.658045	5.427233	0.000000			
4	Ge	2.490876	4.439458	2.769112	0.000000		
5	Ge	2.490876	4.439458	2.769112	2.991324	0.000000	
6	Ge	2.490876	4.439458	2.769112	4.514037	3.380607	
7	Ge	2.552760	2.812373	4.427804	2.715852	2.715852	
8	Ge	2.450798	2.659425	4.405553	2.884046	4.596584	
9	Ge	2.552760	2.812373	4.427804	4.779345	4.779345	
10	Ge	2.450798	2.659425	4.405553	4.596584	2.884046	
11	Ge	2.490876	4.439458	2.769112	3.380607	4.514037	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.779345	0.000000				
8	Ge	4.596584	3.133921	0.000000			
9	Ge	2.715852	4.575003	3.133921	0.000000		
10	Ge	2.884046	3.133921	4.282672	3.133921	0.000000	
11	Ge	2.991324	4.779345	2.884046	2.715852	4.596584	0.000000



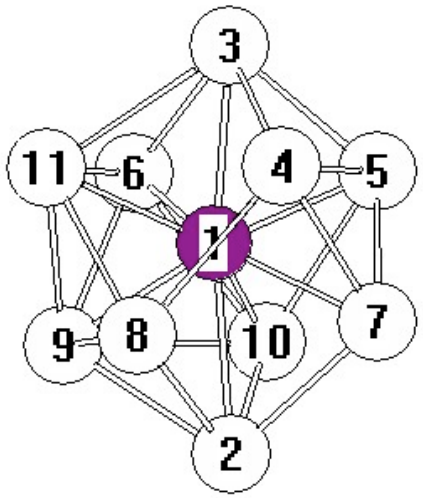
0-4 APT – C_{2v} [7] **[16]**

- 21900.9898823 (+32.58 kcal/mol) ** i -18 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.805118	0.000000				
3	Ge	2.629597	5.418492	0.000000			
4	Ge	2.472723	4.332394	2.682934	0.000000		
5	Ge	2.472723	4.332394	2.682934	3.105297	0.000000	
6	Ge	2.502155	4.529968	2.941140	4.556480	3.460977	
7	Ge	2.576636	2.750366	4.260762	2.658621	2.658621	
8	Ge	2.463427	2.644697	4.432629	2.956217	4.673913	
9	Ge	2.571207	2.845909	4.615622	4.756254	4.756254	
10	Ge	2.463427	2.644697	4.432629	4.673913	2.956217	
11	Ge	2.502155	4.529968	2.941140	3.460977	4.556480	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.847664	0.000000				
8	Ge	4.485749	3.309337	0.000000			
9	Ge	2.743052	4.567054	2.920751	0.000000		
10	Ge	2.860805	3.309337	4.220608	2.920751	0.000000	
11	Ge	2.828439	4.847664	2.860805	2.743052	4.485749	0.000000



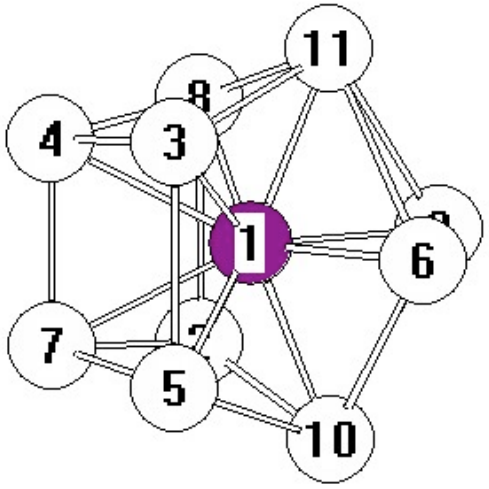
0-4 APT – C_{2v} [7] (r-18) → C_s [7] [15]

- 21900.9901865 (+32.39 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.553319	0.000000				
3	Ge	2.553765	4.870110	0.000000			
4	Ge	2.715942	3.732056	2.540409	0.000000		
5	Ge	2.555603	3.862207	2.969983	3.728390	0.000000	
6	Ge	2.519276	4.594607	3.360233	4.918842	3.348890	
7	Ge	2.716649	2.540642	3.735184	2.516005	2.540453	
8	Ge	2.555409	2.972024	3.857051	2.539832	4.871255	
9	Ge	2.519541	3.350544	4.599298	4.909903	4.611178	
10	Ge	2.556503	2.733926	4.641595	4.941178	2.728263	
11	Ge	2.556597	4.640598	2.734392	3.536258	4.647824	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.910982	0.000000				
8	Ge	4.608044	3.732641	0.000000			
9	Ge	2.580590	4.915128	3.345245	0.000000		
10	Ge	2.950882	3.529258	4.650021	2.981972	0.000000	
11	Ge	2.979332	4.945418	2.727267	2.952849	4.751947	0.000000



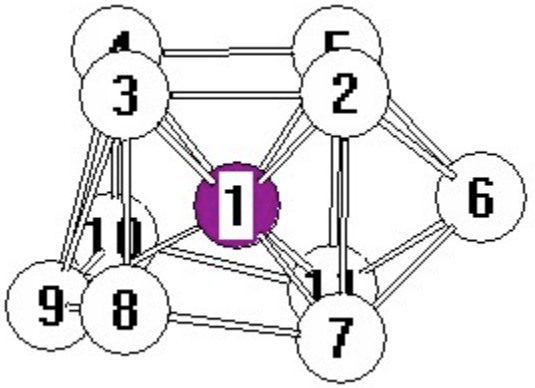
0-4 APT – C_{2v} [9] (r-46, r-33) → C_1 [9] [22]

- 21900.9590763 (+51.91 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.393207	0.000000				
3	Ge	2.453122	2.565222	0.000000			
4	Ge	2.454247	3.708686	2.676796	0.000000		
5	Ge	2.395960	2.684599	3.710561	2.563203	0.000000	
6	Ge	2.848921	2.587456	4.647368	4.643210	2.583672	
7	Ge	2.291050	2.862069	3.803861	4.735432	4.022726	
8	Ge	2.751328	3.627319	2.540446	4.299761	5.022842	
9	Ge	2.445568	4.546387	3.153916	3.140148	4.536740	
10	Ge	2.763328	5.025865	4.314074	2.538290	3.613576	
11	Ge	2.292094	4.019767	4.735261	3.804627	2.863666	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.628033	0.000000				
8	Ge	4.857655	2.687258	0.000000			
9	Ge	5.144780	3.639502	2.422107	0.000000		
10	Ge	4.848601	4.551078	4.520814	2.421567	0.000000	
11	Ge	2.620507	2.970432	4.535322	3.625040	2.683812	0.000000



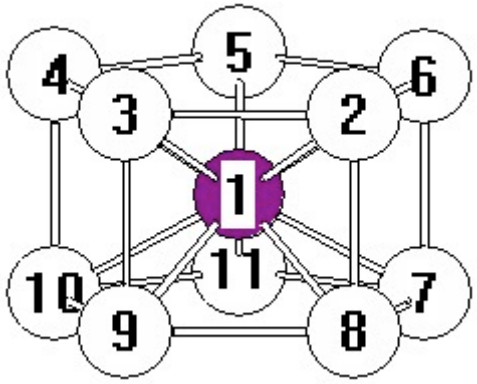
0-5 APP – D_{5d} [1] (ra-106) → C_1 [1] [14]

- 21901.0000565 (+26.19 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.472510	0.000000				
3	Ge	2.473480	2.526499	0.000000			
4	Ge	2.473173	4.087506	2.526188	0.000000		
5	Ge	2.471849	4.087387	4.087618	2.526283	0.000000	
6	Ge	2.472494	2.526827	4.088589	4.088222	2.526397	
7	Ge	2.471849	3.516963	4.763984	4.763340	3.515374	
8	Ge	2.473173	2.445954	3.517692	4.764566	4.763340	
9	Ge	2.473480	3.514634	2.445259	3.517692	4.763984	
10	Ge	2.472510	4.762320	3.514634	2.445954	3.516963	
11	Ge	2.472494	4.764103	4.763616	3.516210	2.446042	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.446042	0.000000				
8	Ge	3.516210	2.526283	0.000000			
9	Ge	4.763616	4.087618	2.526188	0.000000		
10	Ge	4.764103	4.087387	4.087506	2.526499	0.000000	
11	Ge	3.517635	2.526397	4.088222	4.088589	2.526827	0.000000



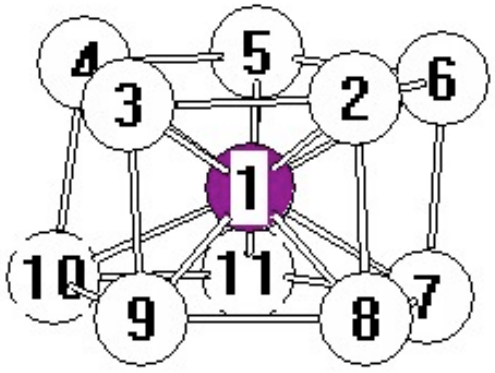
0-5 APP – D_{5d} [1] (rb-101) → C_2 [1] [10]

- 21901.0231901 (+11.68 kcal/mol) ** i -10 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.376347	0.000000				
3	Ge	2.610229	2.549663	0.000000			
4	Ge	2.377154	3.802855	2.551019	0.000000		
5	Ge	2.511833	4.005224	4.319556	2.506104	0.000000	
6	Ge	2.513318	2.505053	4.320672	4.009397	2.571916	
7	Ge	2.433154	3.483870	4.843154	4.652947	3.532657	
8	Ge	2.582821	2.468172	3.588327	4.766009	4.898840	
9	Ge	2.359385	3.457583	2.473358	3.456617	4.696570	
10	Ge	2.583202	4.766250	3.590904	2.468317	3.573025	
11	Ge	2.434427	4.652855	4.845186	3.485306	2.460200	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.460075	0.000000				
8	Ge	3.572546	2.566423	0.000000			
9	Ge	4.697782	3.861488	2.527731	0.000000		
10	Ge	4.900679	4.184414	4.371391	2.527724	0.000000	
11	Ge	3.533334	2.500000	4.186318	3.863343	2.567316	0.000000



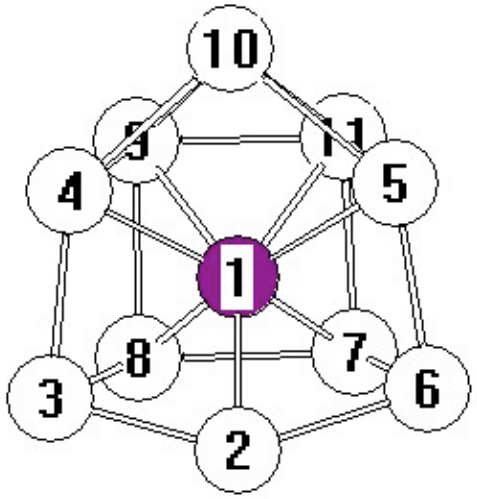
0-5 APP – D_{5d} [1] (rb-101, r-10) → C_1 [1] [9]

- 21901.0232003 (+11.67 kcal/mol) ** i -1 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.394187	0.000000				
3	Ge	2.649187	2.530700	0.000000			
4	Ge	2.445388	3.663841	2.560685	0.000000		
5	Ge	2.445388	3.663841	4.897171	3.875990	0.000000	
6	Ge	2.649187	2.530700	4.495672	4.897171	2.560685	
7	Ge	2.544429	3.672347	4.242117	4.853920	3.685353	
8	Ge	2.544429	3.672347	2.534063	3.685353	4.853920	
9	Ge	2.600515	4.816766	3.703754	2.795597	4.166247	
10	Ge	2.768635	4.780025	4.657325	2.571379	2.571379	
11	Ge	2.600515	4.816766	4.978518	4.166247	2.795597	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.534063	0.000000				
8	Ge	4.242117	2.574494	0.000000			
9	Ge	4.978518	3.611141	2.588866	0.000000		
10	Ge	4.657325	4.641489	4.641489	2.745147	0.000000	
11	Ge	3.703754	2.588866	3.611141	2.461888	2.745147	0.000000



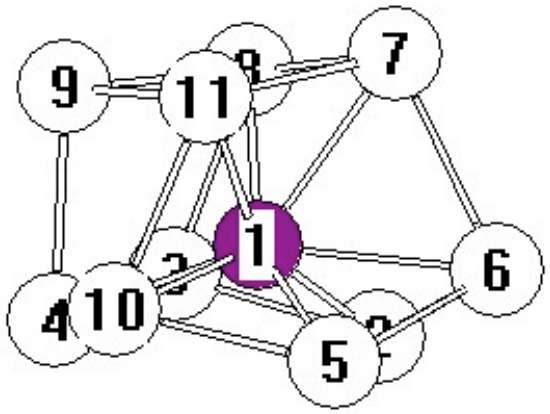
0-5 APP – C_{2h} [5] (ra-159) → C_s [5] [13]

- 21901.0227492 (+11.95 kcal/mol) ** i -55 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.407834	0.000000				
3	Ge	2.755555	2.489402	0.000000			
4	Ge	2.400374	3.818241	2.618899	0.000000		
5	Ge	2.408055	3.653875	4.874237	3.823272	0.000000	
6	Ge	2.653519	2.556417	4.582850	4.929925	2.555133	
7	Ge	2.609119	3.756128	4.510787	4.787023	3.753727	
8	Ge	2.520446	3.236744	2.536149	3.673370	4.829463	
9	Ge	2.734211	4.672849	3.401468	2.559163	4.663250	
10	Ge	2.757173	4.872371	4.802403	2.621571	2.491268	
11	Ge	2.521551	4.830354	4.838501	3.682743	3.223584	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.622653	0.000000				
8	Ge	4.008834	2.582936	0.000000			
9	Ge	5.153724	3.656338	2.509083	0.000000		
10	Ge	4.585480	4.516052	4.833179	3.387152	0.000000	
11	Ge	4.001681	2.582754	3.528886	2.507509	2.538634	0.000000



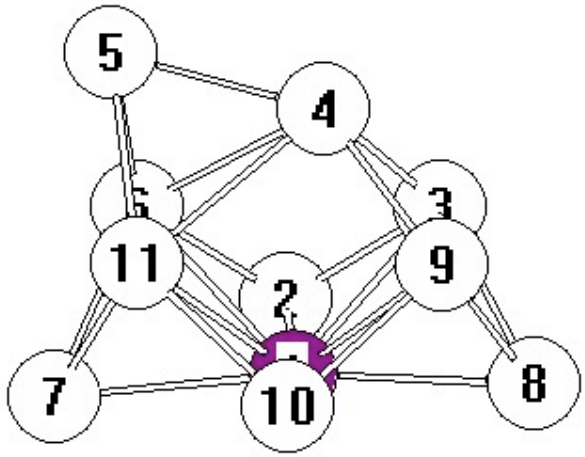
0-5 APP – C_{2h} [5] (ra-159, r-55) → C_1 [5] [8]

- 21901.0252443 (+10.39 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.735839	0.000000				
3	Ge	2.744927	2.524416	0.000000			
4	Ge	3.091739	3.951860	2.489390	0.000000		
5	Ge	4.256656	4.849228	4.542626	2.476426	0.000000	
6	Ge	2.781652	2.557297	3.439316	2.917107	2.546616	
7	Ge	2.730427	3.827019	4.985348	4.516787	4.038670	
8	Ge	2.710201	3.910817	2.504865	3.986889	6.128368	
9	Ge	2.745520	4.756703	2.982531	2.488799	4.542301	
10	Ge	2.735324	5.447865	4.755395	3.949508	4.846574	
11	Ge	2.780764	4.670129	4.495034	2.919339	2.546618	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.525994	0.000000				
8	Ge	5.009904	5.426965	0.000000			
9	Ge	4.494490	4.988082	2.503701	0.000000		
10	Ge	4.670669	3.831544	3.909233	2.523982	0.000000	
11	Ge	2.803375	2.525178	5.010454	3.443051	2.557483	0.000000



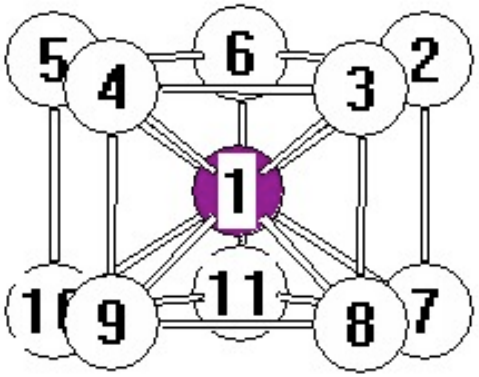
0-5 APP – C_{2h} [9] (ra-96, r-81) → C_1 [9] [24]

- 21900.9561242 (+53.76 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.510770	0.000000				
3	Ge	2.614925	2.684774	0.000000			
4	Ge	2.615049	4.216164	2.671145	0.000000		
5	Ge	2.512078	3.973147	4.228539	2.687602	0.000000	
6	Ge	2.640198	2.528089	4.377415	4.371489	2.525819	
7	Ge	2.512078	2.687458	3.739142	4.962809	4.796642	
8	Ge	2.615049	3.745595	2.526466	3.680364	4.962809	
9	Ge	2.614925	4.960493	3.673004	2.526466	3.739142	
10	Ge	2.510770	4.796748	4.960493	3.745595	2.687458	
11	Ge	2.640198	3.647871	5.061992	5.064086	3.645456	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.645456	0.000000				
8	Ge	5.064086	2.687602	0.000000			
9	Ge	5.061992	4.228539	2.671145	0.000000		
10	Ge	3.647871	3.973147	4.216164	2.684774	0.000000	
11	Ge	2.572196	2.525819	4.371489	4.377415	2.528089	0.000000



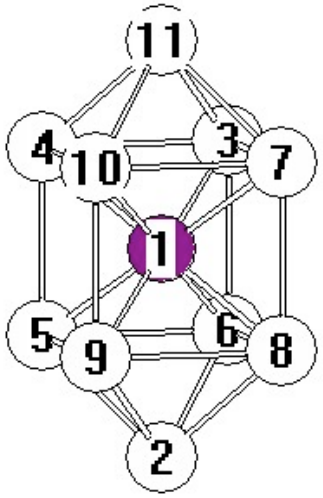
0-5 APP – C_{2h} [9] (rb-41) → C_2 [9] [23]

- 21900.9570582 (+53.17 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.036559	0.000000				
3	Ge	2.410563	4.840890	0.000000			
4	Ge	2.410563	4.840890	2.791590	0.000000		
5	Ge	2.410563	2.574643	3.930685	2.767184	0.000000	
6	Ge	2.410563	2.574643	2.767184	3.930685	2.791590	
7	Ge	2.410563	4.840890	2.791590	3.947905	4.821126	
8	Ge	2.410563	2.574643	3.930685	4.821126	3.947905	
9	Ge	2.410563	2.574643	4.821126	3.930685	2.791590	
10	Ge	2.410563	4.840890	3.947905	2.791590	3.930685	
11	Ge	3.036559	6.073118	2.574643	2.574643	4.840890	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.930685	0.000000				
8	Ge	2.791590	2.767184	0.000000			
9	Ge	3.947905	3.930685	2.791590	0.000000		
10	Ge	4.821126	2.791590	3.930685	2.767184	0.000000	
11	Ge	4.840890	2.574643	4.840890	4.840890	2.574643	0.000000



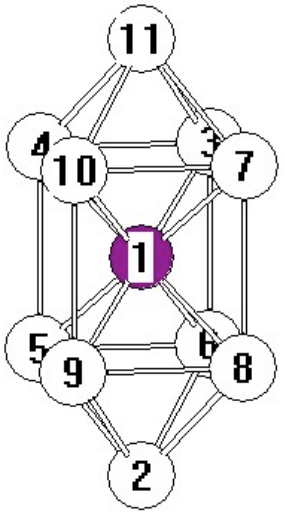
0-8 CBO – D_{4h} [3] [18]

- 21900.9676405 (+46.53 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.354303	0.000000				
3	Ge	2.427026	5.246317	0.000000			
4	Ge	2.427026	5.246317	2.644044	0.000000		
5	Ge	2.427026	2.599955	4.070732	3.095140	0.000000	
6	Ge	2.427026	2.599955	3.095140	4.070732	2.644044	
7	Ge	2.427026	5.246317	2.644044	3.739243	4.854053	
8	Ge	2.427026	2.599955	4.070732	4.854053	3.739243	
9	Ge	2.427026	2.599955	4.854053	4.070732	2.644044	
10	Ge	2.427026	5.246317	3.739243	2.644044	4.070732	
11	Ge	3.354303	6.708606	2.599955	2.599955	5.246317	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.070732	0.000000				
8	Ge	2.644044	3.095140	0.000000			
9	Ge	3.739243	4.070732	2.644044	0.000000		
10	Ge	4.854053	2.644044	4.070732	3.095140	0.000000	
11	Ge	5.246317	2.599955	5.246317	5.246317	2.599955	0.000000



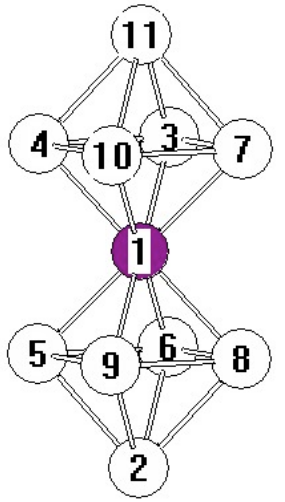
0-8 CBO – D_{4h} [7] **[19]**

- 21900.9673868 (+46.69 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	3.721799	0.000000				
3	Ge	2.549629	5.813172	0.000000			
4	Ge	2.549629	5.813172	2.545669	0.000000		
5	Ge	2.549629	2.629034	4.418371	3.611312	0.000000	
6	Ge	2.549629	2.629034	3.611312	4.418371	2.545669	
7	Ge	2.549629	5.813172	2.545669	3.600119	5.099258	
8	Ge	2.549629	2.629034	4.418371	5.099258	3.600119	
9	Ge	2.549629	2.629034	5.099258	4.418371	2.545669	
10	Ge	2.549629	5.813172	3.600119	2.545669	4.418371	
11	Ge	3.721799	7.443598	2.629034	2.629034	5.813172	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.418371	0.000000				
8	Ge	2.545669	3.611312	0.000000			
9	Ge	3.600119	4.418371	2.545669	0.000000		
10	Ge	5.099258	2.545669	4.418371	3.611312	0.000000	
11	Ge	5.813172	2.629034	5.813172	5.813172	2.629034	0.000000



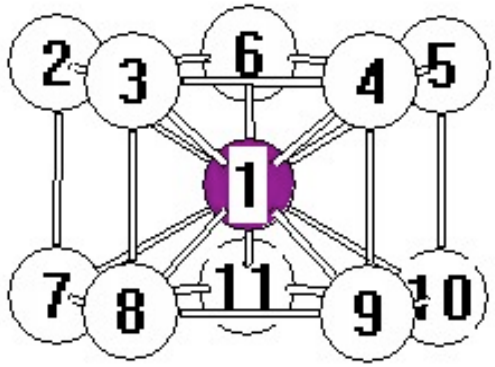
0-8 CBO – D_{4h} [9] **[21]**

- 21900.9608262 (+50.81 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.472911	0.000000				
3	Ge	2.472911	2.526774	0.000000			
4	Ge	2.472911	4.088406	2.526774	0.000000		
5	Ge	2.472911	4.088406	4.088406	2.526774	0.000000	
6	Ge	2.472911	2.526774	4.088406	4.088406	2.526774	
7	Ge	2.472911	2.445698	3.516536	4.764084	4.764084	
8	Ge	2.472911	3.516536	2.445698	3.516536	4.764084	
9	Ge	2.472911	4.764084	3.516536	2.445698	3.516536	
10	Ge	2.472911	4.764084	4.764084	3.516536	2.445698	
11	Ge	2.472911	3.516536	4.764084	4.764084	3.516536	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.516536	0.000000				
8	Ge	4.764084	2.526774	0.000000			
9	Ge	4.764084	4.088406	2.526774	0.000000		
10	Ge	3.516536	4.088406	4.088406	2.526774	0.000000	
11	Ge	2.445698	2.526774	4.088406	4.088406	2.526774	0.000000



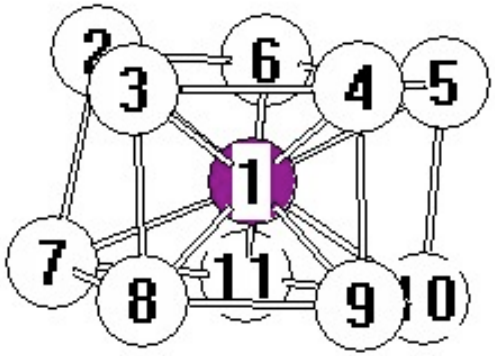
0-9 PPG – D_{5h} [1] [12]

- 21901.0231164 (+11.72 kcal/mol) ** i -14 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.359414	0.000000				
3	Ge	2.628262	2.551572	0.000000			
4	Ge	2.374280	3.745087	2.564251	0.000000		
5	Ge	2.498709	3.948790	4.341811	2.502375	0.000000	
6	Ge	2.537091	2.507283	4.385746	4.033949	2.579322	
7	Ge	2.609315	2.479846	3.571151	4.777299	4.910607	
8	Ge	2.349568	3.472281	2.483335	3.472296	4.679003	
9	Ge	2.586130	4.748204	3.579709	2.475690	3.573594	
10	Ge	2.442904	4.648196	4.866200	3.500412	2.466293	
11	Ge	2.410148	3.483573	4.829336	4.636695	3.530028	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.583526	0.000000				
8	Ge	4.706557	2.531063	0.000000			
9	Ge	4.927763	4.417871	2.519587	0.000000		
10	Ge	3.550500	4.245232	3.840291	2.578873	0.000000	
11	Ge	2.469146	2.576620	3.787845	4.165301	2.499575	0.000000



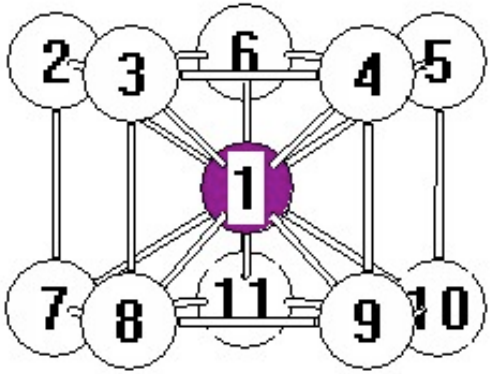
0-9 PPG – D_{5h} [1] (ra-14) → C_1 [1] [11]

- 21901.0231498 (+11.70 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.505257	0.000000				
3	Ge	2.505257	2.510487	0.000000			
4	Ge	2.505257	4.062054	2.510487	0.000000		
5	Ge	2.505257	4.062054	4.062054	2.510487	0.000000	
6	Ge	2.505257	2.510487	4.062054	4.062054	2.510487	
7	Ge	2.505257	2.619729	3.628433	4.833556	4.833556	
8	Ge	2.505257	3.628433	2.619729	3.628433	4.833556	
9	Ge	2.505257	4.833556	3.628433	2.619729	3.628433	
10	Ge	2.505257	4.833556	4.833556	3.628433	2.619729	
11	Ge	2.505257	3.628433	4.833556	4.833556	3.628433	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.628433	0.000000				
8	Ge	4.833556	2.510487	0.000000			
9	Ge	4.833556	4.062054	2.510487	0.000000		
10	Ge	3.628433	4.062054	4.062054	2.510487	0.000000	
11	Ge	2.619729	2.510487	4.062054	4.062054	2.510487	0.000000



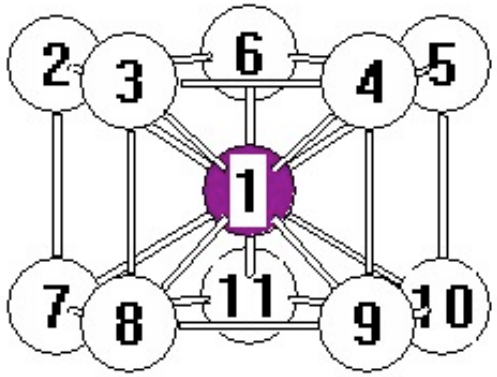
0-9 PPG – D_{5h} [5] [17]

- 21900.9752508 (+41.76 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.505692	0.000000				
3	Ge	2.505692	2.527144	0.000000			
4	Ge	2.505692	4.089005	2.527144	0.000000		
5	Ge	2.505692	4.089005	4.089005	2.527144	0.000000	
6	Ge	2.505692	2.527144	4.089005	4.089005	2.527144	
7	Ge	2.505692	2.574654	3.607673	4.832060	4.832060	
8	Ge	2.505692	3.607673	2.574654	3.607673	4.832060	
9	Ge	2.505692	4.832060	3.607673	2.574654	3.607673	
10	Ge	2.505692	4.832060	4.832060	3.607673	2.574654	
11	Ge	2.505692	3.607673	4.832060	4.832060	3.607673	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.607673	0.000000				
8	Ge	4.832060	2.527144	0.000000			
9	Ge	4.832060	4.089005	2.527144	0.000000		
10	Ge	3.607673	4.089005	4.089005	2.527144	0.000000	
11	Ge	2.574654	2.527144	4.089005	4.089005	2.527144	0.000000



0-9 PPG – D_{5h} [7] [20]

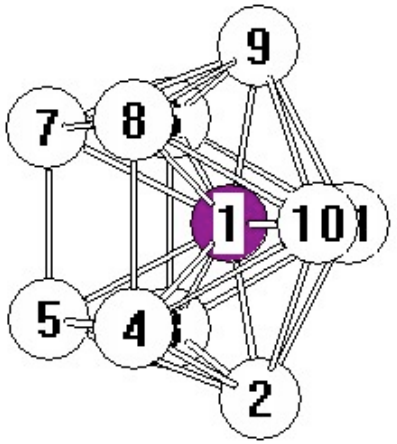
- 21900.9610447 (+50.67 kcal/mol)

$Mn@Ge_{10}^{z}$ – solvent THF

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.302092	0.000000				
3	Ge	2.681026	2.672049	0.000000			
4	Ge	2.681026	2.672049	4.160403	0.000000		
5	Ge	2.661106	2.930571	2.476619	2.476619	0.000000	
6	Ge	2.673881	4.395020	2.690451	4.951871	3.568192	
7	Ge	2.667701	4.450505	3.576884	3.576884	2.461673	
8	Ge	2.673881	4.395020	4.951871	2.690451	3.568192	
9	Ge	2.301133	4.540750	4.401509	4.401509	4.442516	
10	Ge	2.244563	3.046079	4.736091	2.726548	4.290715	
11	Ge	2.244563	3.046079	2.726548	4.736091	4.290715	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.479224	0.000000				
8	Ge	4.154044	2.479224	0.000000			
9	Ge	2.667658	2.932414	2.667658	0.000000		
10	Ge	4.735112	4.302250	2.729049	3.061054	0.000000	
11	Ge	2.729049	4.302250	4.735112	3.061054	3.604578	0.000000



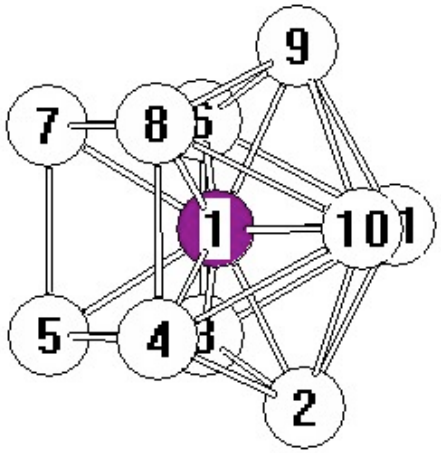
0-3 CCD – C_s [1] [6]

- 21901.0818930 (+14.36 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.509327	0.000000				
3	Ge	2.480829	2.700873	0.000000			
4	Ge	2.480829	2.700873	4.041134	0.000000		
5	Ge	2.508123	3.359034	2.623324	2.623324	0.000000	
6	Ge	2.486513	4.424382	2.708827	4.880075	3.746241	
7	Ge	2.500200	4.809475	3.745819	3.745819	2.633749	
8	Ge	2.486513	4.424382	4.880075	2.708827	3.746241	
9	Ge	2.510434	4.540007	4.432090	4.432090	4.805061	
10	Ge	2.509014	2.857680	4.492498	2.931727	4.627178	
11	Ge	2.509014	2.857680	2.931727	4.492498	4.627178	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.629709	0.000000				
8	Ge	4.077416	2.629709	0.000000			
9	Ge	2.707190	3.320195	2.707190	0.000000		
10	Ge	4.494566	4.611234	2.917117	2.864226	0.000000	
11	Ge	2.917117	4.611234	4.494566	2.864226	2.867394	0.000000



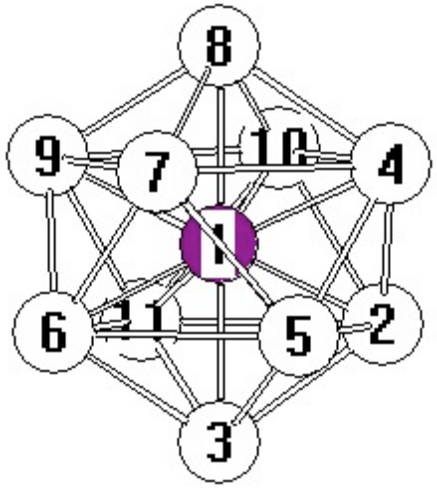
0-3 CCD – C_s [5] [3]

- 21901.0955444 (+5.80 kcal/mol) ** i -56 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.511371	0.000000				
3	Ge	2.485982	2.695469	0.000000			
4	Ge	2.511028	2.737134	4.200428	0.000000		
5	Ge	2.510241	3.241165	2.687687	2.728523	0.000000	
6	Ge	2.511734	4.559932	2.690957	4.724516	3.252230	
7	Ge	2.512115	4.724395	4.191041	3.256937	2.729567	
8	Ge	2.488049	4.219719	4.973793	2.691811	4.188915	
9	Ge	2.512554	4.696099	4.220764	4.559910	4.718043	
10	Ge	2.512721	2.741219	4.231075	3.217392	4.712461	
11	Ge	2.513239	3.199443	2.702728	4.703304	4.562667	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.728828	0.000000				
8	Ge	4.203906	2.687013	0.000000			
9	Ge	2.734489	3.229548	2.695880	0.000000		
10	Ge	4.698867	4.561019	2.700836	3.195370	0.000000	
11	Ge	3.208765	4.707689	4.231909	2.739513	2.743580	0.000000



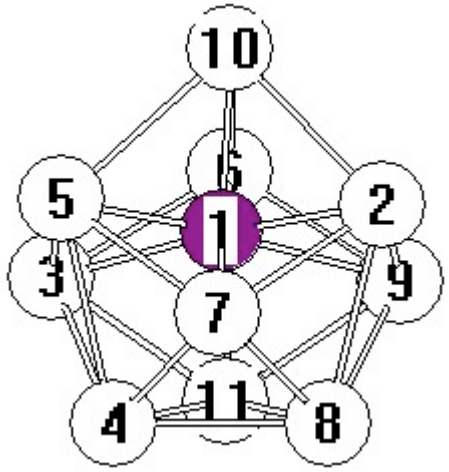
0-3 CCD – C_s [5] (r-56) → C_1 [5] [2]

- 21901.0988948 (+3.70 kcal/mol)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.311155	0.000000				
3	Ge	2.540008	4.847081	0.000000			
4	Ge	2.712382	4.275065	2.637300	0.000000		
5	Ge	2.289716	3.898463	2.661892	2.861774	0.000000	
6	Ge	2.305098	3.881514	2.658618	4.284214	3.907760	
7	Ge	2.552015	2.649714	4.245853	2.638735	2.655954	
8	Ge	2.705191	2.815478	4.234034	2.618644	4.272630	
9	Ge	2.583877	2.640547	4.253832	4.266720	4.871319	
10	Ge	2.247267	2.821068	3.880317	4.777832	2.902398	
11	Ge	2.708057	4.252783	2.630240	2.626501	4.283992	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.853410	0.000000				
8	Ge	4.250300	2.627236	0.000000			
9	Ge	2.642308	4.254346	2.626577	0.000000		
10	Ge	2.839596	3.863609	4.714441	3.811119	0.000000	
11	Ge	2.826875	4.245688	2.606361	2.630637	4.730560	0.000000



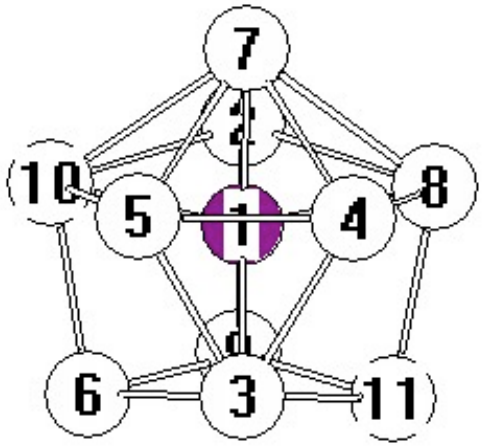
0-4 APT – C_1 [1] [1]

- 21901.1047842 (**+0.00 kcal/mol**)

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.319933	0.000000				
3	Ge	2.586413	4.832322	0.000000			
4	Ge	2.754047	4.724208	2.624402	0.000000		
5	Ge	2.754047	4.724208	2.624402	2.574180	0.000000	
6	Ge	2.726683	4.186249	2.466399	4.518862	3.325187	
7	Ge	2.398749	3.245348	4.160027	2.705377	2.705377	
8	Ge	2.348762	3.138622	3.752220	2.627085	4.327109	
9	Ge	2.354394	2.748336	3.436803	4.709125	4.709125	
10	Ge	2.348762	3.138622	3.752220	4.327109	2.627085	
11	Ge	2.726683	4.186249	2.466399	3.325187	4.518862	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.678050	0.000000				
8	Ge	4.827742	3.018218	0.000000			
9	Ge	2.563162	4.672885	3.563305	0.000000		
10	Ge	2.569424	3.018218	4.592645	3.563305	0.000000	
11	Ge	3.637371	4.678050	2.569424	2.563162	4.827742	0.000000



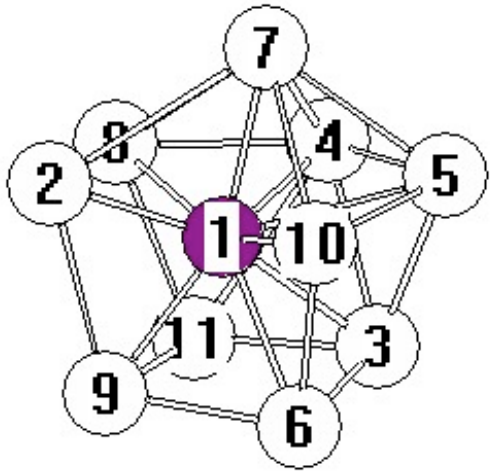
0-4 APT – C_{2v} [3] (rb-377) → C_s [3] [5]

- 21901.0910206 (+8.64 kcal/mol) ** i -56 **

Charge 1+

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.306417	0.000000				
3	Ge	2.608822	4.834247	0.000000			
4	Ge	2.629850	4.317383	2.662873	0.000000		
5	Ge	2.791548	4.828811	2.626316	2.573328	0.000000	
6	Ge	2.618545	4.238505	2.513952	4.496218	3.599914	
7	Ge	2.412784	3.099771	4.248994	2.803233	2.711161	
8	Ge	2.509006	2.621286	4.061853	2.596732	4.462245	
9	Ge	2.368573	2.741914	3.530688	4.489072	4.891390	
10	Ge	2.309850	3.584593	3.592260	4.188576	2.586421	
11	Ge	2.680650	3.953695	2.483596	2.923665	4.400179	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.651355	0.000000				
8	Ge	4.889784	3.126990	0.000000			
9	Ge	2.566153	4.657695	3.474861	0.000000		
10	Ge	2.533495	2.909702	4.689984	3.788555	0.000000	
11	Ge	3.621346	4.603385	2.612392	2.576038	4.765857	0.000000



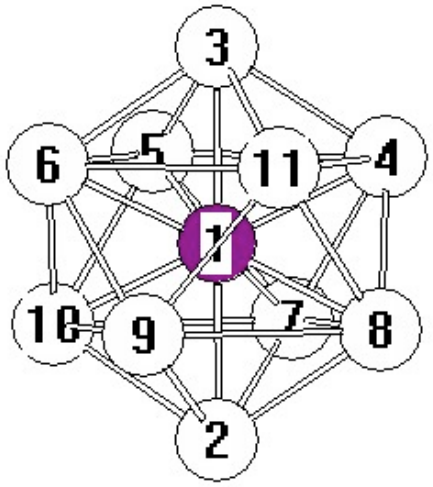
0-4 APT – C_{2v} [3] (rb-377, r-56) → C_1 [3] [4]

- 21901.0949805 (+6.15 kcal/mol)

Charge 1+

		1	2	3	4	5	6
1	Mn	0.000000					
2	Ge	2.486476	0.000000				
3	Ge	2.486876	4.973352	0.000000			
4	Ge	2.512541	4.211436	2.693659	0.000000		
5	Ge	2.512541	4.211436	2.693659	3.225601	0.000000	
6	Ge	2.512541	4.211436	2.693659	4.561689	3.225601	
7	Ge	2.512614	2.693099	4.212081	2.737074	2.737074	
8	Ge	2.512614	2.693099	4.212081	2.737074	4.712211	
9	Ge	2.512614	2.693099	4.212081	4.712211	4.712211	
10	Ge	2.512614	2.693099	4.212081	4.712211	2.737074	
11	Ge	2.512541	4.211436	2.693659	3.225601	4.561689	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.712211	0.000000				
8	Ge	4.712211	3.225420	0.000000			
9	Ge	2.737074	4.561433	3.225420	0.000000		
10	Ge	2.737074	3.225420	4.561433	3.225420	0.000000	
11	Ge	3.225601	4.712211	2.737074	2.737074	4.712211	0.000000



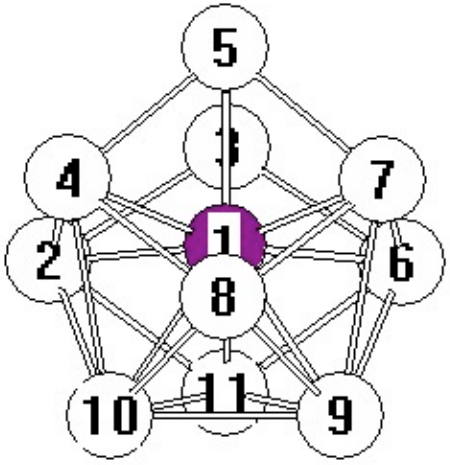
0-4 APT – C_{4v} [5] **[2]**

- 21901.0988895 (+3.70 kcal/mol)

Charge 0

		1	2	3	4	5	6
1	Mn	0.000000					
2	Ge	2.495986	0.000000				
3	Ge	2.395745	2.678524	0.000000			
4	Ge	2.395745	2.678524	3.811801	0.000000		
5	Ge	2.411293	3.700071	2.643517	2.643517	0.000000	
6	Ge	2.495986	4.282552	2.678524	4.847548	3.700071	
7	Ge	2.395745	4.847548	3.811801	3.811801	2.643517	
8	Ge	2.495986	4.282552	4.847548	2.678524	3.700071	
9	Ge	2.552175	4.400636	4.421256	4.421256	4.676438	
10	Ge	2.552175	2.721476	4.421256	2.983778	4.676438	
11	Ge	2.552175	2.721476	2.983778	4.421256	4.676438	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.678524	0.000000				
8	Ge	4.282552	2.678524	0.000000			
9	Ge	2.721476	2.983778	2.721476	0.000000		
10	Ge	4.400636	4.421256	2.721476	2.792533	0.000000	
11	Ge	2.721476	4.421256	4.400636	2.792533	2.792533	0.000000



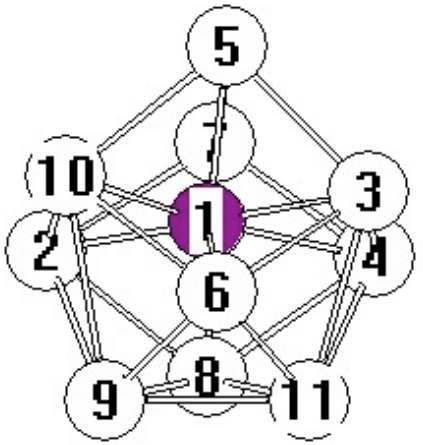
0-3 CCD – C_{3v} [4] **[1]**

- 21901.3059896 (**+0.00 kcal/mol**)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.402937	0.000000				
3	Ge	2.400962	4.803854	0.000000			
4	Ge	2.527025	4.194023	2.599496	0.000000		
5	Ge	2.268910	3.811202	2.687552	3.677061	0.000000	
6	Ge	2.527505	4.195357	2.599739	4.181471	3.676039	
7	Ge	2.324259	2.719988	3.859933	2.622636	2.784645	
8	Ge	2.673663	2.682421	4.326155	2.682289	4.749403	
9	Ge	2.673752	2.683053	4.326437	4.297847	4.748696	
10	Ge	2.324387	2.720343	3.860778	4.841724	2.785022	
11	Ge	2.652080	4.197712	2.844610	2.634233	4.604050	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.841946	0.000000				
8	Ge	4.297917	3.002277	0.000000			
9	Ge	2.682719	4.437861	2.696650	0.000000		
10	Ge	2.622303	3.961770	4.436811	2.999870	0.000000	
11	Ge	2.633950	4.309559	2.618184	2.618368	4.308366	0.000000



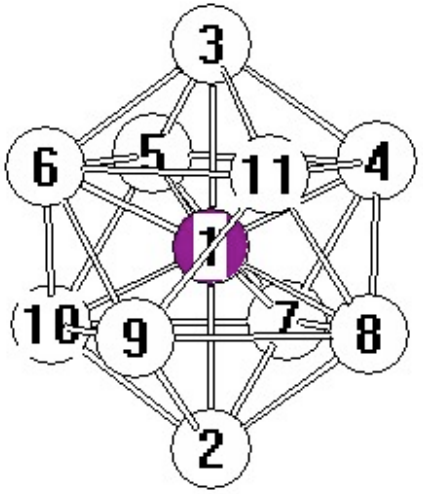
0-4 APT – C_{4v} [2] (r-54) → C_1 [2] [2]

- 21901.3035899 (+1.51 kcal/mol)

Charge 0

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.615448	0.000000				
3	Ge	2.615364	5.230812	0.000000			
4	Ge	2.493521	4.315673	2.736994	0.000000		
5	Ge	2.493521	4.315673	2.736994	3.189070	0.000000	
6	Ge	2.493521	4.315673	2.736994	4.510026	3.189070	
7	Ge	2.493320	2.736974	4.315411	2.740125	2.740125	
8	Ge	2.493320	2.736974	4.315411	2.740125	4.678677	
9	Ge	2.493320	2.736974	4.315411	4.678677	4.678677	
10	Ge	2.493320	2.736974	4.315411	4.678677	2.740125	
11	Ge	2.493521	4.315673	2.736994	3.189070	4.510026	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.678677	0.000000				
8	Ge	4.678677	3.188837	0.000000			
9	Ge	2.740125	4.509696	3.188837	0.000000		
10	Ge	2.740125	3.188837	4.509696	3.188837	0.000000	
11	Ge	3.189070	4.678677	2.740125	2.740125	4.678677	0.000000



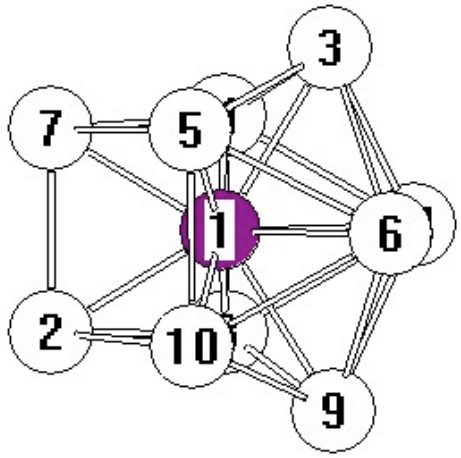
0-4 APT – C_{4v} [6] [3]

- 21901.2695166 (+22.89 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.411549	0.000000				
3	Ge	2.582517	4.847299	0.000000			
4	Ge	2.437873	3.787026	2.697430	0.000000		
5	Ge	2.437873	3.787026	2.697430	4.109566	0.000000	
6	Ge	2.598081	4.667801	2.723824	4.346206	2.796498	
7	Ge	2.410521	2.470049	3.548273	2.810782	2.810782	
8	Ge	2.436422	2.800913	4.344458	2.632236	4.864710	
9	Ge	2.591454	3.578077	4.402602	4.336399	4.336399	
10	Ge	2.436422	2.800913	4.344458	4.864710	2.632236	
11	Ge	2.598081	4.667801	2.723824	2.796498	4.346206	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.662650	0.000000				
8	Ge	4.342794	3.795682	0.000000			
9	Ge	2.718195	4.862631	2.688158	0.000000		
10	Ge	2.808958	3.795682	4.072628	2.688158	0.000000	
11	Ge	2.693497	4.662650	2.808958	2.718195	4.342794	0.000000



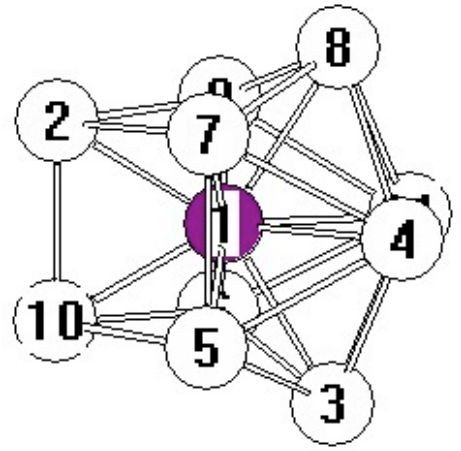
0-4 APT – C_{2v} [5] (ra-397) → C_s [5] [3]

- 21901.4380704 (+3.25 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.408522	0.000000				
3	Ge	2.585315	4.848546	0.000000			
4	Ge	2.600180	4.668321	2.718100	0.000000		
5	Ge	2.438096	3.788907	2.694758	2.793825	0.000000	
6	Ge	2.438096	3.788907	2.694758	4.343418	4.104334	
7	Ge	2.435455	2.804908	4.340966	2.806151	2.631627	
8	Ge	2.590941	3.578170	4.399232	2.720011	4.336715	
9	Ge	2.435455	2.804908	4.340966	4.343332	4.864643	
10	Ge	2.410739	2.471662	3.552160	4.662831	2.810858	
11	Ge	2.600180	4.668321	2.718100	2.694668	4.343418	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.864643	0.000000				
8	Ge	4.336715	2.689917	0.000000			
9	Ge	2.631627	4.078442	2.689917	0.000000		
10	Ge	2.810858	3.797556	4.864062	3.797556	0.000000	
11	Ge	2.793825	4.343332	2.720011	2.806151	4.662831	0.000000



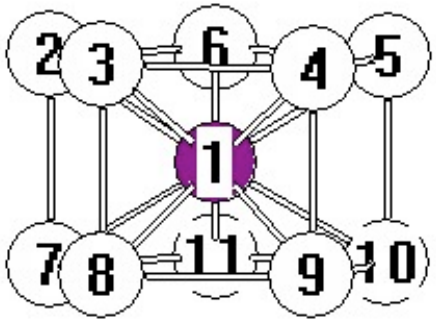
0-4 APT – C_{2v} [5] (rb-331) → C_s [5] [3]

- 21901.4380729 (+3.25 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.462599	0.000000				
3	Ge	2.483159	2.444461	0.000000			
4	Ge	2.499249	4.052864	2.537672	0.000000		
5	Ge	2.499249	4.052864	4.134329	2.647242	0.000000	
6	Ge	2.483159	2.444461	4.024149	4.134329	2.537672	
7	Ge	2.462599	2.525940	3.513815	4.765595	4.765595	
8	Ge	2.483159	3.513815	2.522430	3.565982	4.834162	
9	Ge	2.499249	4.765595	3.565982	2.488256	3.633085	
10	Ge	2.499249	4.765595	4.834162	3.633085	2.488256	
11	Ge	2.483159	3.513815	4.749361	4.834162	3.565982	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.513815	0.000000				
8	Ge	4.749361	2.444461	0.000000			
9	Ge	4.834162	4.052864	2.537672	0.000000		
10	Ge	3.565982	4.052864	4.134329	2.647242	0.000000	
11	Ge	2.522430	2.444461	4.024149	4.134329	2.537672	0.000000



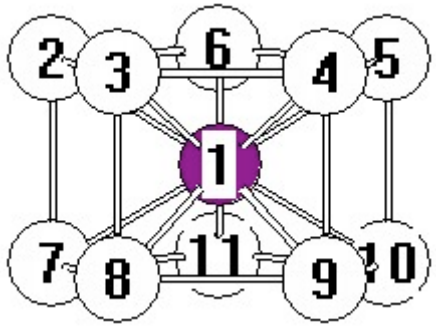
0-9 PPG – C_{2v} [1] **[2]**

- 21901.4394391 (+2.39 kcal/mol)

Charge 1-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.483276	0.000000				
3	Ge	2.483276	2.518504	0.000000			
4	Ge	2.483276	4.075026	2.518504	0.000000		
5	Ge	2.483276	4.075026	4.075026	2.518504	0.000000	
6	Ge	2.483276	2.518504	4.075026	4.075026	2.518504	
7	Ge	2.483276	2.511510	3.556761	4.786807	4.786807	
8	Ge	2.483276	3.556761	2.511510	3.556761	4.786807	
9	Ge	2.483276	4.786807	3.556761	2.511510	3.556761	
10	Ge	2.483276	4.786807	4.786807	3.556761	2.511510	
11	Ge	2.483276	3.556761	4.786807	4.786807	3.556761	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.556761	0.000000				
8	Ge	4.786807	2.518504	0.000000			
9	Ge	4.786807	4.075026	2.518504	0.000000		
10	Ge	3.556761	4.075026	4.075026	2.518504	0.000000	
11	Ge	2.511510	2.518504	4.075026	4.075026	2.518504	0.000000



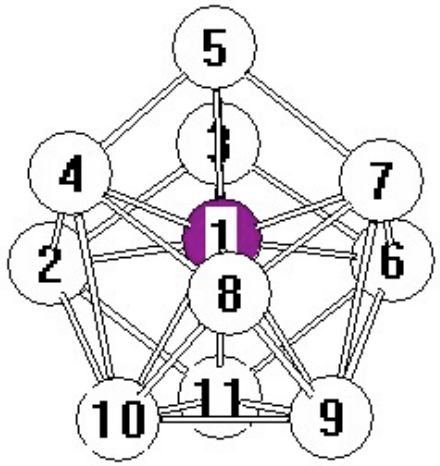
0-9 PPG – D_{5h} [3] **[1]**

- 21901.4432545 (**+0.00 kcal/mol**)

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.433213	0.000000				
3	Ge	2.400080	2.714652	0.000000			
4	Ge	2.400080	2.714652	3.867239	0.000000		
5	Ge	2.349359	3.614056	2.588070	2.588070	0.000000	
6	Ge	2.486766	4.204533	2.683771	4.853754	3.725957	
7	Ge	2.362688	4.778639	3.818557	3.818557	2.773705	
8	Ge	2.486766	4.204533	4.853754	2.683771	3.725957	
9	Ge	2.627659	4.264283	4.463433	4.463433	4.773578	
10	Ge	2.620751	2.714268	4.489419	3.147373	4.720354	
11	Ge	2.620751	2.714268	3.147373	4.489419	4.720354	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.633838	0.000000				
8	Ge	4.229452	2.633838	0.000000			
9	Ge	2.747282	3.043455	2.747282	0.000000		
10	Ge	4.326581	4.382940	2.740518	2.615025	0.000000	
11	Ge	2.740518	4.382940	4.326581	2.615025	2.650193	0.000000



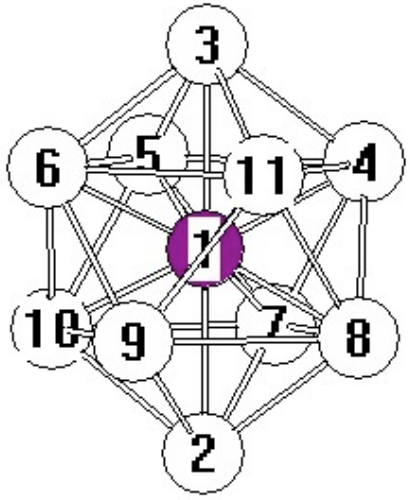
0-3 CCD – C_s [4] [3]

- 21901.5674968 (+8.41 kcal/mol) ** i -33 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.644442	0.000000				
3	Ge	2.644476	5.288918	0.000000			
4	Ge	2.427883	4.314844	2.675370	0.000000		
5	Ge	2.427883	4.314844	2.675370	3.072710	0.000000	
6	Ge	2.427883	4.314844	2.675370	4.345467	3.072710	
7	Ge	2.427921	2.675889	4.314583	2.731100	2.731100	
8	Ge	2.427921	2.675889	4.314583	2.731100	4.562137	
9	Ge	2.427921	2.675889	4.314583	4.562137	4.562137	
10	Ge	2.427921	2.675889	4.314583	4.562137	2.731100	
11	Ge	2.427883	4.314844	2.675370	3.072710	4.345467	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	4.562137	0.000000				
8	Ge	4.562137	3.073130	0.000000			
9	Ge	2.731100	4.346062	3.073130	0.000000		
10	Ge	2.731100	3.073130	4.346062	3.073130	0.000000	
11	Ge	3.072710	4.562137	2.731100	2.731100	4.562137	0.000000



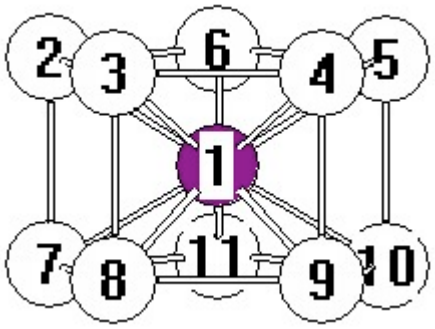
0-4 APT – C_{4v} [4] [4]

- 21901.5178809 (+39.54 kcal/mol) ** i -33 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.488614	0.000000				
3	Ge	2.488884	2.523274	0.000000			
4	Ge	2.488645	4.082814	2.523556	0.000000		
5	Ge	2.488645	4.082814	4.083139	2.523502	0.000000	
6	Ge	2.488884	2.523274	4.083091	4.083139	2.523556	
7	Ge	2.488614	2.518451	3.565207	4.797179	4.797179	
8	Ge	2.488884	3.565207	2.518925	3.565541	4.797579	
9	Ge	2.488645	4.797179	3.565541	2.518829	3.565468	
10	Ge	2.488645	4.797179	4.797579	3.565468	2.518829	
11	Ge	2.488884	3.565207	4.797564	4.797579	3.565541	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.565207	0.000000				
8	Ge	4.797564	2.523274	0.000000			
9	Ge	4.797579	4.082814	2.523556	0.000000		
10	Ge	3.565541	4.082814	4.083139	2.523502	0.000000	
11	Ge	2.518925	2.523274	4.083091	4.083139	2.523556	0.000000



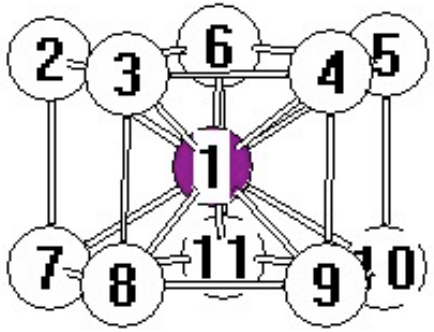
0-9 PPG – C_s [4] [2]

- 21901.5776779 (+2.02 kcal/mol) ** i -37 **

Charge 2-

		1	2	3	4	5	
1	Mn	0.000000					
2	Ge	2.448770	0.000000				
3	Ge	2.468466	2.603712	0.000000			
4	Ge	2.543995	4.109938	2.503945	0.000000		
5	Ge	2.581984	4.112226	4.061866	2.456986	0.000000	
6	Ge	2.527526	2.595721	4.151619	4.057056	2.507552	
7	Ge	2.448770	2.561536	3.644611	4.847084	4.859851	
8	Ge	2.527526	3.664837	2.576890	3.652428	4.882256	
9	Ge	2.581984	4.859851	3.551509	2.600283	3.661006	
10	Ge	2.543995	4.847084	4.744584	3.491426	2.600283	
11	Ge	2.468466	3.644611	4.837406	4.744584	3.551509	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.664837	0.000000				
8	Ge	4.933424	2.595721	0.000000			
9	Ge	4.882256	4.112226	2.507552	0.000000		
10	Ge	3.652428	4.109938	4.057056	2.456986	0.000000	
11	Ge	2.576890	2.603712	4.151619	4.061866	2.503945	0.000000



0-9 PPG – C_s [4] (r-37, ra-217) → C_2 [4] [1]

- 21901.5808958 (**+0.00 kcal/mol**) ** i -15 **

Complete Gaussian 09 reference (Reference 30)

M. J. Frisch; G. W. Trucks; H. B. Schlegel; G. E. Scuseria; M. A. Robb; J. R.Cheeseman; G. Scalmani; V. Barone; B. Mennucci; G. A. Petersson; H. Nakatsuji; M. Caricato; X. Li; H. P. Hratchian; A. F. Izmaylov; J. Bloino; G. Zheng; J. L. Sonnenberg; M. Hada; M. Ehara; K. Toyota; R. Fukuda; J. Hasegawa; M. Ishida; T. Nakajima; Y. Honda; O. Kitao; H. Nakai; T. Vreven; J. A. Montgomery; Jr.; J. E. Peralta; F. Ogliaro; M. Bearpark; J. J. Heyd; E. Brothers; K. N. Kudin; V. N. Staroverov; R. Kobayashi; J.Normand; K. Raghavachari; A. Rendell; J. C. Burant; S. S. Iyengar; J. Tomasi; M.Cossi; N. Rega; J. M. Millam; M. Klene; J. E. Knox; J. B. Cross; V. Bakken; C.Adamo; J. Jaramillo; R. Gomperts; R. E. Stratmann; O. Yazyev; A. J. Austin; R.Cammi; C. Pomelli; J. W. Ochterski; R. L. Martin; K. Morokuma; V. G. Zakrzewski; G. A. Voth; P. Salvador; J. J. Dannenberg; S. Dapprich; A. D. Daniels; O. Farkas; J. B. Foresman; J. V. Ortiz; J. Cioslowski; and D. J. Fox, Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.