Density Functional Theory Study of Twelve-Atom Germanium Clusters: Conflict between the Wade-Mingos Rules and Optimum Vertex Degrees

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Supporting Information

Figure S1. Ge_{12}^{z} Initial Structures

Table S1. Optimized Ge_{12}^{z} Structures with their Energies and Geometries

Table S2. Energies of the Bonding Molecular Orbitals of Ge_{12} and Ge_{12}^{2-}

Figure S1. Ge_{12}^{z} Initial Structures

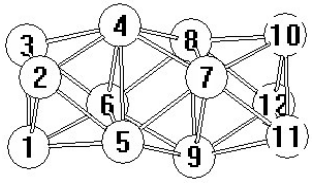
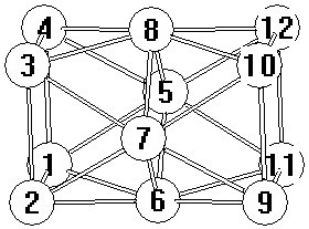
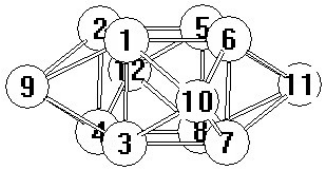
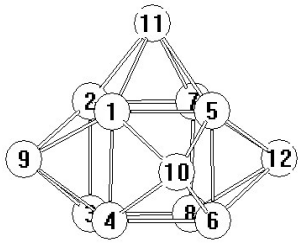
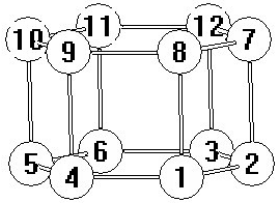
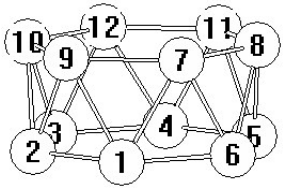
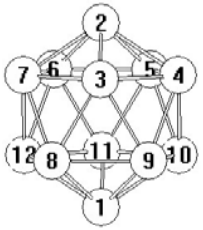
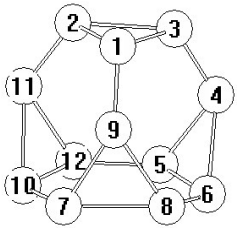
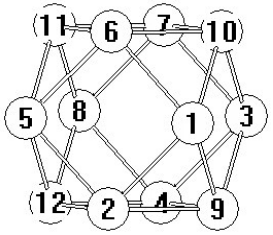
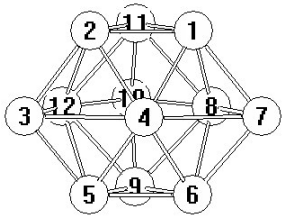
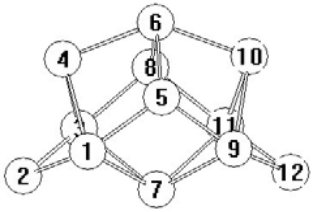
 1-1 – D_{3d}	 1-2 – D_{4h}	 2-1 – D_{4h}	 2-2 – C_{2v}
 3-1 – D_{6h}	 3-2 – D_{6d}	 4-1 – I_h	 5-1 – S_4
 6-1 – O_h	 7-1 – D_{3h}	 7-2 – C_{2v}	

Table S1. Optimized Ge_{12}^{z} Structures with their Energies and Geometries

Ge_{12} – 1-1_OctTrp-D_{3d}

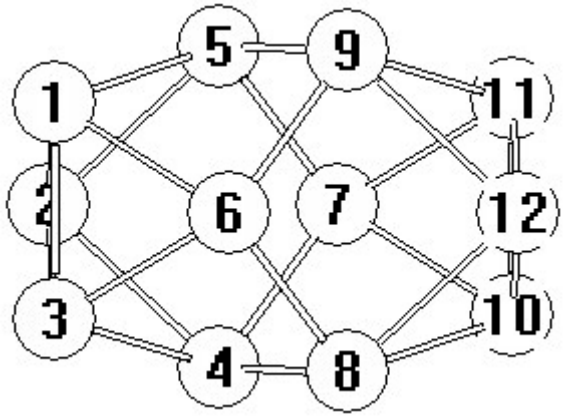
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.503832	0.000000			
3	Ge	2.503832	2.503832	0.000000		
4	Ge	4.106828	2.743283	2.743283	0.000000	
5	Ge	2.743283	2.743283	4.106828	3.730456	0.000000
6	Ge	2.743283	4.106828	2.743283	3.730456	3.730456
7	Ge	4.610944	3.452589	4.610944	2.569709	2.569709
8	Ge	4.610944	4.610944	3.452589	2.569709	4.529868
9	Ge	3.452589	4.610944	4.610944	4.529868	2.569709
10	Ge	6.087126	5.548327	5.548327	3.452589	4.610944
11	Ge	5.548327	5.548327	6.087126	4.610944	3.452589
12	Ge	5.548327	6.087126	5.548327	4.610944	4.610944

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.529868	0.000000			
8	Ge	2.569709	3.730456	0.000000		
9	Ge	2.569709	3.730456	3.730456	0.000000	
10	Ge	4.610944	2.743283	2.743283	4.106828	0.000000
11	Ge	4.610944	2.743283	4.106828	2.743283	2.503832
12	Ge	3.452589	4.106828	2.743283	2.743283	2.503832

		11	12
11	Ge	0.000000	
12	Ge	2.503832	0.000000



1-1 OctTrp – D_{3d} [28-1]

- 24899.9581776 (**+0.00 kcal/mol**)

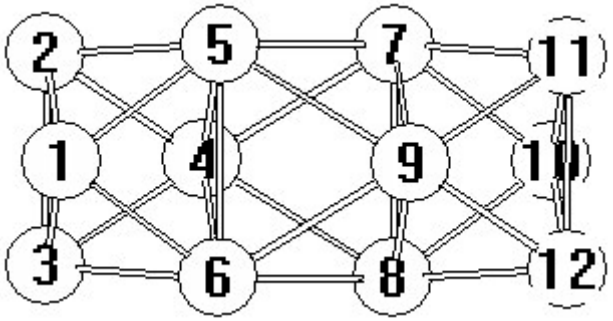
Charge
2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.634977	0.000000			
3	Ge	2.634977	2.634977	0.000000		
4	Ge	3.798027	2.598117	2.598117	0.000000	
5	Ge	2.598117	2.598117	3.798027	2.912660	0.000000
6	Ge	2.598117	3.798027	2.598117	2.912660	2.912660
7	Ge	5.164213	4.358245	5.164213	2.860627	2.860627
8	Ge	5.164213	5.164213	4.358245	2.860627	4.082496
9	Ge	4.358245	5.164213	5.164213	4.082496	2.860627
10	Ge	7.083209	6.574856	6.574856	4.358245	5.164213
11	Ge	6.574856	6.574856	7.083209	5.164213	4.358245
12	Ge	6.574856	7.083209	6.574856	5.164213	5.164213

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.082496	0.000000			
8	Ge	2.860627	2.912660	0.000000		
9	Ge	2.860627	2.912660	2.912660	0.000000	
10	Ge	5.164213	2.598117	2.598117	3.798027	0.000000
11	Ge	5.164213	2.598117	3.798027	2.598117	2.634977
12	Ge	4.358245	3.798027	2.598117	2.598117	2.634977

		11	12
11	Ge	0.000000	
12	Ge	2.634977	0.000000



1-1 OctTrp – D_{3d} [HE]

- 24900.3282201 (+76.28 kcal/mol)

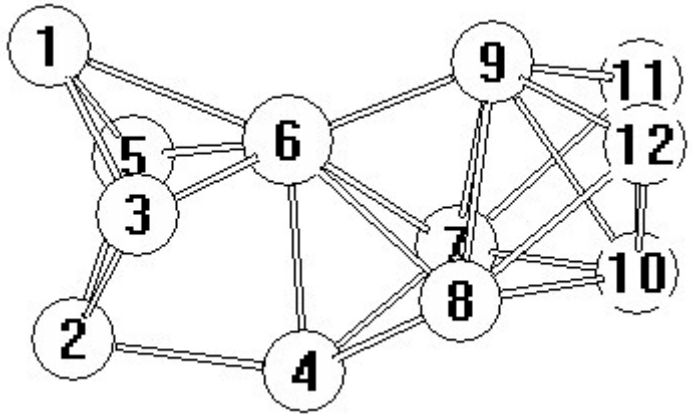
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.503240	0.000000			
3	Ge	2.550324	2.567148	0.000000		
4	Ge	4.872390	2.707737	3.377036	0.000000	
5	Ge	2.549374	2.566542	3.295738	3.373126	0.000000
6	Ge	2.992655	3.422906	2.465684	2.735957	2.466200
7	Ge	5.661437	4.760393	4.980042	2.578234	3.881870
8	Ge	5.662800	4.762182	3.887482	2.579970	4.976260
9	Ge	5.143479	5.855940	4.677439	4.246684	4.670669
10	Ge	7.342028	6.582557	6.133361	4.022571	6.127813
11	Ge	7.165680	7.351843	6.874043	5.289950	5.935780
12	Ge	7.167511	7.354764	5.944366	5.292145	6.868683

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.928296	0.000000			
8	Ge	2.924949	2.940553	0.000000		
9	Ge	2.542805	2.924781	2.926729	0.000000	
10	Ge	4.349667	2.543060	2.543374	3.012887	0.000000
11	Ge	4.512080	2.886087	4.357747	2.584962	2.631502
12	Ge	4.509469	4.355933	2.888584	2.585004	2.630053

		11	12
11	Ge	0.000000	
12	Ge	3.620188	0.000000



1-1.1 OctTrp – D_{3d} → C_1 [HE]

- 24898.5826392 (+21.67 kcal/mol)

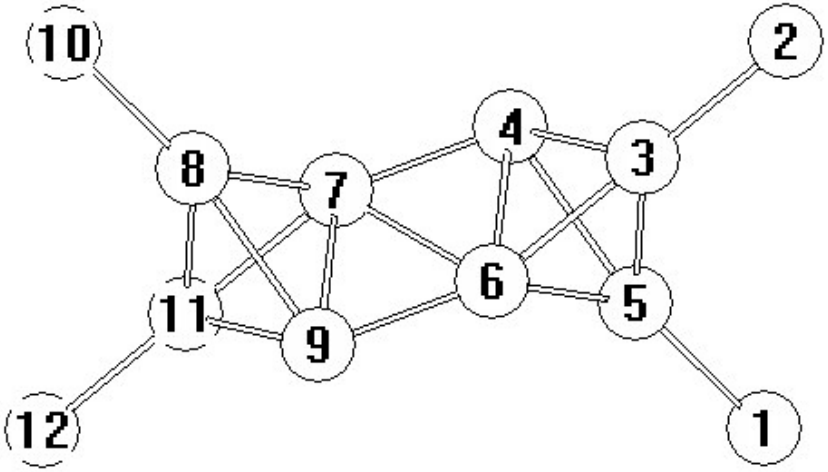
Charge 6+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	6.677070	0.000000			
3	Ge	4.910810	2.724625	0.000000		
4	Ge	5.146403	5.150208	2.826333	0.000000	
5	Ge	2.723862	4.908827	2.498824	2.824560	0.000000
6	Ge	5.045684	5.047814	2.501041	2.979919	2.500908
7	Ge	6.578992	6.579623	4.125108	2.598214	4.126762
8	Ge	8.828377	7.828978	5.800449	4.926470	6.316828
9	Ge	7.156825	7.156170	4.924135	4.959251	4.926470
10	Ge	11.437528	9.287819	7.825001	7.156825	8.828377
11	Ge	7.825001	8.829095	6.314772	4.924135	5.800449
12	Ge	9.287819	11.440133	8.829095	7.156170	7.828978

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.582072	0.000000			
8	Ge	4.126762	2.500908	0.000000		
9	Ge	2.598214	2.979919	2.824560	0.000000	
10	Ge	6.578992	5.045684	2.723862	5.146403	0.000000
11	Ge	4.125108	2.501041	2.498824	2.826333	4.910810
12	Ge	6.579623	5.047814	4.908827	5.150208	6.677070

		11	12
11	Ge	0.000000	
12	Ge	2.724625	0.000000



1-1.1 OctTrp – D_{3d} → C_i [18-1]

- 24897.0455610 (**+0.00 kcal/mol**)

Ge_{12} – 1-2_CubDbl-D_{4h}

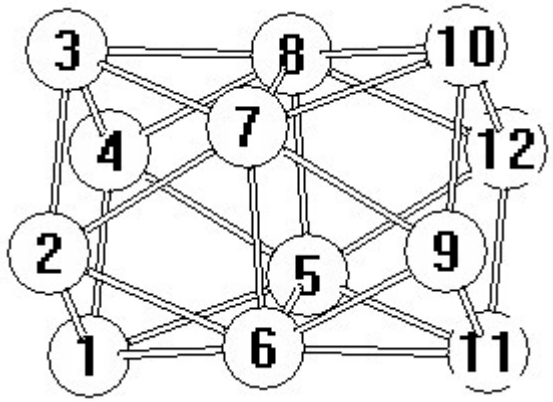
Charge 6-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.634334	0.000000			
3	Ge	3.725511	2.634334	0.000000		
4	Ge	2.634334	3.725511	2.634334	0.000000	
5	Ge	2.759224	4.197635	4.197635	2.759224	0.000000
6	Ge	2.759224	2.759224	4.197635	4.197635	2.686027
7	Ge	4.197635	2.759224	2.759224	4.197635	3.798616
8	Ge	4.197635	4.197635	2.759224	2.759224	2.686027
9	Ge	5.394231	4.707230	5.394231	6.003119	4.197635
10	Ge	6.003119	5.394231	4.707230	5.394231	4.197635
11	Ge	4.707230	5.394231	6.003119	5.394231	2.759224
12	Ge	5.394231	6.003119	5.394231	4.707230	2.759224

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.686027	0.000000			
8	Ge	3.798616	2.686027	0.000000		
9	Ge	2.759224	2.759224	4.197635	0.000000	
10	Ge	4.197635	2.759224	2.759224	2.634334	0.000000
11	Ge	2.759224	4.197635	4.197635	2.634334	3.725511
12	Ge	4.197635	4.197635	2.759224	3.725511	2.634334

		11	12
11	Ge	0.000000	
12	Ge	2.634334	0.000000



1-2 CubDbl – D_{4h} [30-3]

- 24898.9569362 (+54.20 kcal/mol)

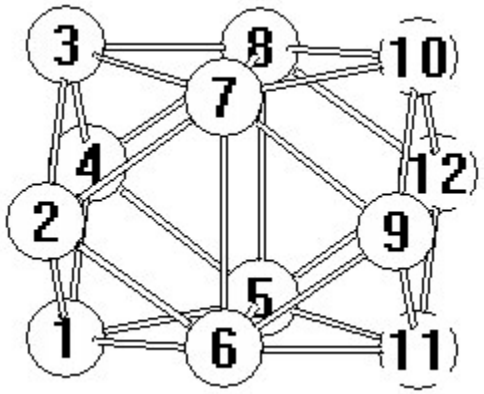
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.570082	0.000000			
3	Ge	3.634645	2.570082	0.000000		
4	Ge	2.570082	3.634645	2.570082	0.000000	
5	Ge	2.678501	4.306157	4.306157	2.678501	0.000000
6	Ge	2.678501	2.678501	4.306157	4.306157	3.127850
7	Ge	4.306157	2.678501	2.678501	4.306157	4.423448
8	Ge	4.306157	4.306157	2.678501	2.678501	3.127850
9	Ge	5.026182	4.319396	5.026182	5.645159	4.306157
10	Ge	5.645159	5.026182	4.319396	5.026182	4.306157
11	Ge	4.319396	5.026182	5.645159	5.026182	2.678501
12	Ge	5.026182	5.645159	5.026182	4.319396	2.678501

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	3.127850	0.000000			
8	Ge	4.423448	3.127850	0.000000		
9	Ge	2.678501	2.678501	4.306157	0.000000	
10	Ge	4.306157	2.678501	2.678501	2.570082	0.000000
11	Ge	2.678501	4.306157	4.306157	2.570082	3.634645
12	Ge	4.306157	4.306157	2.678501	3.634645	2.570082

		11	12
11	Ge	0.000000	
12	Ge	2.570082	0.000000



1-2 CubDbl – D_{4h} [HE]

- 24899.9157237 (+26.64 kcal/mol)

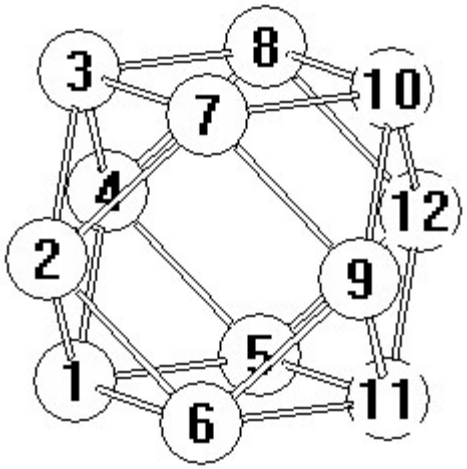
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.604439	0.000000			
3	Ge	3.683233	2.604439	0.000000		
4	Ge	2.604439	3.683233	2.604439	0.000000	
5	Ge	2.605409	4.509794	4.509794	2.605409	0.000000
6	Ge	2.605409	2.605409	4.509794	4.509794	3.678859
7	Ge	4.509794	2.605409	2.605409	4.509794	5.202692
8	Ge	4.509794	4.509794	2.605409	2.605409	3.678859
9	Ge	4.516824	3.690338	4.516824	5.213904	4.509794
10	Ge	5.213904	4.516824	3.690338	4.516824	4.509794
11	Ge	3.690338	4.516824	5.213904	4.516824	2.605409
12	Ge	4.516824	5.213904	4.516824	3.690338	2.605409

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	3.678859	0.000000			
8	Ge	5.202692	3.678859	0.000000		
9	Ge	2.605409	2.605409	4.509794	0.000000	
10	Ge	4.509794	2.605409	2.605409	2.604439	0.000000
11	Ge	2.605409	4.509794	4.509794	2.604439	3.683233
12	Ge	4.509794	4.509794	2.605409	3.683233	2.604439

		11	12
11	Ge	0.000000	
12	Ge	2.604439	0.000000



1-2 CubDbl – D_{4h} [HE]

- 24900.3671613 (+51.84 kcal/mol)

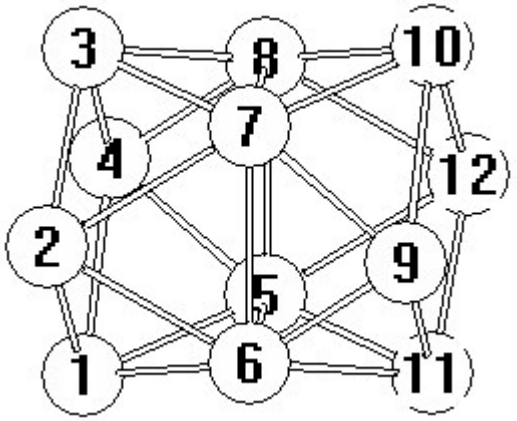
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.512728	0.000000			
3	Ge	3.951139	2.512380	0.000000		
4	Ge	2.954311	3.739082	2.954085	0.000000	
5	Ge	2.626163	4.152006	4.268125	2.425469	0.000000
6	Ge	2.430668	2.748511	4.148652	4.174985	2.861538
7	Ge	4.151089	2.750272	2.430246	4.175680	4.049426
8	Ge	4.267392	4.152029	2.627200	2.424709	2.863556
9	Ge	4.724583	4.212336	4.724164	5.499142	4.175680
10	Ge	5.644351	5.120525	4.030126	4.724583	4.151089
11	Ge	4.030126	5.120179	5.643414	4.724164	2.430246
12	Ge	5.120525	5.762678	5.120179	4.212336	2.750272

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.863556	0.000000			
8	Ge	4.047081	2.861538	0.000000		
9	Ge	2.424709	2.425469	4.174985	0.000000	
10	Ge	4.267392	2.626163	2.430668	2.954311	0.000000
11	Ge	2.627200	4.268125	4.148652	2.954085	3.951139
12	Ge	4.152029	4.152006	2.748511	3.739082	2.512728

		11	12
11	Ge	0.000000	
12	Ge	2.512380	0.000000



1-2.1 CubDbl – $D_{4h}{}^{T}$ → C_i [HE]

- 24900.3234025 (+37.30 kcal/mol)

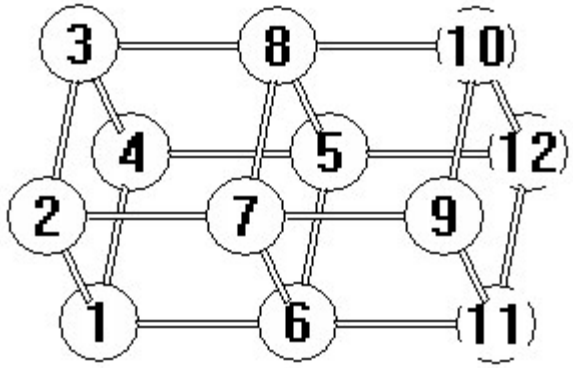
Charge 2+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.458082	0.000000			
3	Ge	3.476253	2.458082	0.000000		
4	Ge	2.458082	3.476253	2.458082	0.000000	
5	Ge	3.522067	4.297238	3.529224	2.528661	0.000000
6	Ge	2.528661	3.522067	4.297238	3.529224	2.455620
7	Ge	3.529224	2.528661	3.522067	4.297238	3.472771
8	Ge	4.297238	3.529224	2.528661	3.522067	2.455620
9	Ge	5.623029	5.057300	5.623029	6.136825	4.297238
10	Ge	6.136825	5.623029	5.057300	5.623029	3.529224
11	Ge	5.057300	5.623029	6.136825	5.623029	3.522067
12	Ge	5.623029	6.136825	5.623029	5.057300	2.528661

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.455620	0.000000			
8	Ge	3.472771	2.455620	0.000000		
9	Ge	3.522067	2.528661	3.529224	0.000000	
10	Ge	4.297238	3.522067	2.528661	2.458082	0.000000
11	Ge	2.528661	3.529224	4.297238	2.458082	3.476253
12	Ge	3.529224	4.297238	3.522067	3.476253	2.458082

		11	12
11	Ge	0.000000	
12	Ge	2.458082	0.000000



1-2.1 CubDbl – D_{4h} → C_{4h} [22-3]

- 24899.7656078 (+8.29 kcal/mol)

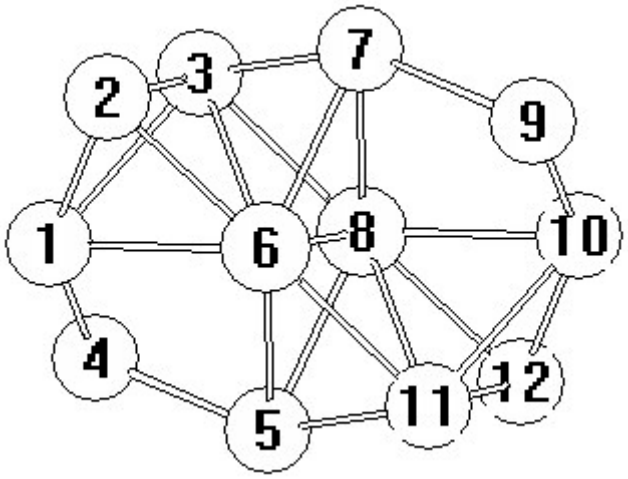
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.503117	0.000000			
3	Ge	2.785680	3.017614	0.000000		
4	Ge	2.623111	4.951043	3.615934	0.000000	
5	Ge	3.362846	4.911911	4.127806	2.549982	0.000000
6	Ge	2.739460	2.555000	3.093914	4.107478	2.864818
7	Ge	4.203047	3.127866	2.489204	5.406203	4.669787
8	Ge	3.798889	4.510460	2.573805	3.438011	2.561559
9	Ge	6.001346	4.829091	4.907389	7.046415	5.406203
10	Ge	6.011802	5.900191	4.758395	6.001346	4.203047
11	Ge	4.758395	5.121761	4.966178	4.907389	2.489204
12	Ge	5.900191	6.783356	5.121761	4.829091	3.127866

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.561559	0.000000			
8	Ge	2.780401	2.864818	0.000000		
9	Ge	3.438011	2.549982	4.107478	0.000000	
10	Ge	3.798889	3.362846	2.739460	2.623111	0.000000
11	Ge	2.573805	4.127806	3.093914	3.615934	2.785680
12	Ge	4.510460	4.911911	2.555000	4.951043	2.503117

		11	12
11	Ge	0.000000	
12	Ge	3.017614	0.000000



1-2.1 CubDbl – D_{4h} → C_i [20-3]

- 24898.6029542 (+8.92 kcal/mol)

Charge 6+

Distance matrix (angstroms):

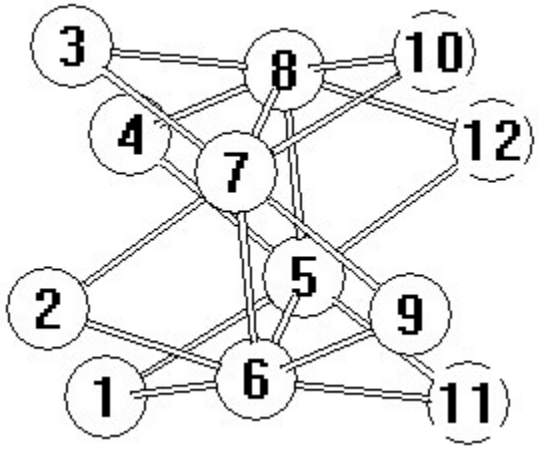
		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.282445	0.000000			
3	Ge	4.642079	3.282445	0.000000		
4	Ge	3.282445	4.642079	3.282445	0.000000	
5	Ge	2.767143	4.515110	4.515110	2.767143	0.000000
6	Ge	2.767143	2.767143	4.515110	4.515110	2.742120
7	Ge	4.515110	2.767143	2.767143	4.515110	3.877943
8	Ge	4.515110	4.515110	2.767143	2.767143	2.742120
9	Ge	5.502155	4.415797	5.502155	6.406883	4.515110
10	Ge	6.406883	5.502155	4.415797	5.502155	4.515110
11	Ge	4.415797	5.502155	6.406883	5.502155	2.767143
12	Ge	5.502155	6.406883	5.502155	4.415797	2.767143

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.742120	0.000000			
8	Ge	3.877943	2.742120	0.000000		
9	Ge	2.767143	2.767143	4.515110	0.000000	
10	Ge	4.515110	2.767143	2.767143	3.282445	0.000000
11	Ge	2.767143	4.515110	4.515110	3.282445	4.642079
12	Ge	4.515110	4.515110	2.767143	4.642079	3.282445

		11	12
11	Ge	0.000000	
12	Ge	3.282445	0.000000

1-2 CubDbl – D_{4h} [HE]

- 24896.8564207 (+118.68 kcal/mol)



Ge_{12} – 2-1_CubTetracap-D_{4h}

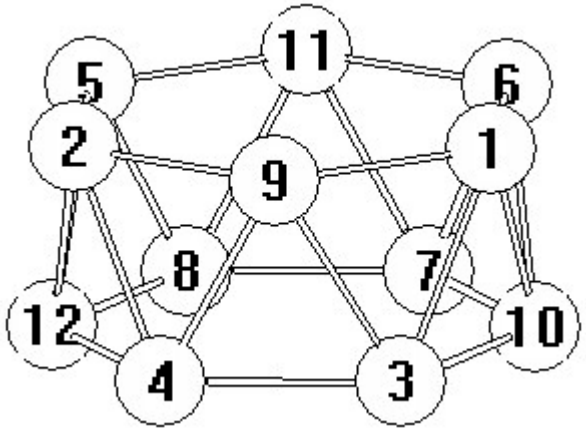
Charge 6-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	4.542368	0.000000			
3	Ge	2.727859	4.399778	0.000000		
4	Ge	4.399778	2.727859	2.623484	0.000000	
5	Ge	5.245548	2.623484	5.592395	4.399778	0.000000
6	Ge	2.623484	5.245548	4.399778	5.592395	4.542368
7	Ge	4.399778	5.592395	4.542368	5.245548	4.399778
8	Ge	5.592395	4.399778	5.245548	4.542368	2.727859
9	Ge	2.622944	2.622944	2.727806	2.727806	4.543892
10	Ge	2.727806	5.592645	2.622944	4.543892	5.592645
11	Ge	4.543892	4.543892	5.592645	5.592645	2.622944
12	Ge	5.592645	2.727806	4.543892	2.622944	2.727806

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.727859	0.000000			
8	Ge	4.399778	2.623484	0.000000		
9	Ge	4.543892	5.592645	5.592645	0.000000	
10	Ge	2.727806	2.622944	4.543892	4.400063	0.000000
11	Ge	2.622944	2.727806	2.727806	5.247648	4.400063
12	Ge	5.592645	4.543892	2.622944	4.400063	5.247648

		11	12
11	Ge	0.000000	
12	Ge	4.400063	0.00000



2-1.1 CubTetracap – D_{4h} → D_{2d} [30-5]

- 24898.9321418 (+69.75 kcal/mol)

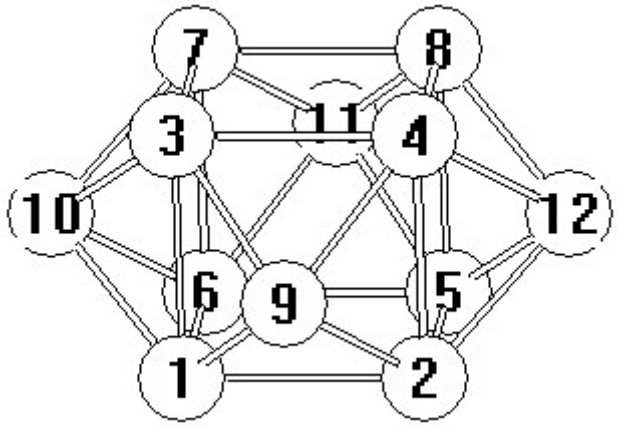
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.759882	0.000000			
3	Ge	2.930523	4.025533	0.000000		
4	Ge	4.025533	2.930523	2.759882	0.000000	
5	Ge	3.903062	2.759882	4.880765	4.025533	0.000000
6	Ge	2.759882	3.903062	4.025533	4.880765	2.759882
7	Ge	4.025533	4.880765	2.759882	3.903062	4.025533
8	Ge	4.880765	4.025533	3.903062	2.759882	2.930523
9	Ge	2.550532	2.550532	2.550532	2.550532	4.771685
10	Ge	2.550532	4.771685	2.550532	4.771685	4.771685
11	Ge	4.771685	4.771685	4.771685	4.771685	2.550532
12	Ge	4.771685	2.550532	4.771685	2.550532	2.550532

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.930523	0.000000			
8	Ge	4.025533	2.759882	0.000000		
9	Ge	4.771685	4.771685	4.771685	0.000000	
10	Ge	2.550532	2.550532	4.771685	4.166925	0.000000
11	Ge	2.550532	2.550532	2.550532	5.892922	4.166925
12	Ge	4.771685	4.771685	2.550532	4.166925	5.892922

		11	12
11	Ge	0.000000	
12	Ge	4.166925	0.000000



2-1 CubTetracap – D_{4h} [T] [HE]

- 24900.3699044 (+50.12 kcal/mol)

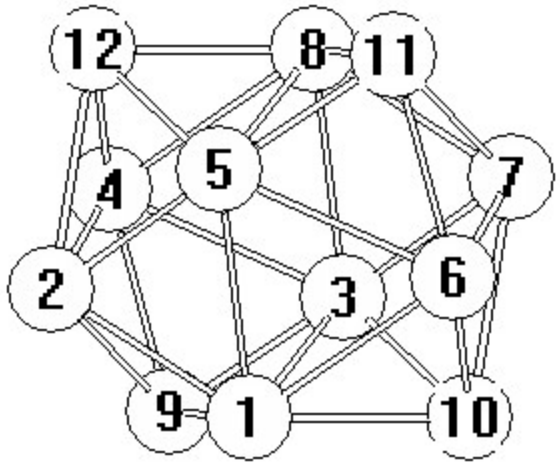
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.725564	0.000000			
3	Ge	2.805375	3.722749	0.000000		
4	Ge	4.168543	2.682918	2.998980	0.000000	
5	Ge	2.881636	2.549327	3.397568	3.612668	0.000000
6	Ge	3.049424	4.864326	3.612668	5.705001	2.998980
7	Ge	4.190432	5.401147	2.549327	4.864326	3.722749
8	Ge	4.561188	4.190432	2.881636	3.049424	2.805375
9	Ge	2.702181	2.802163	2.392783	2.625404	4.155361
10	Ge	2.598749	4.971174	2.488174	5.302329	4.191023
11	Ge	4.507897	4.894362	4.155361	5.157661	2.392783
12	Ge	4.651093	2.803136	4.191023	2.478462	2.488174

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.682918	0.000000			
8	Ge	4.168543	2.725564	0.000000		
9	Ge	5.157661	4.894362	4.507897	0.000000	
10	Ge	2.478462	2.803136	4.651093	3.878068	0.000000
11	Ge	2.625404	2.802163	2.702181	5.868680	4.490571
12	Ge	5.302329	4.971174	2.598749	4.490571	5.997324

		11	12
11	Ge	0.000000	
12	Ge	3.878068	0.000000



2-1.1 CubTetracap – D_{4h} → C_i [24-6]

- 24900.3378197 (+28.25 kcal/mol)

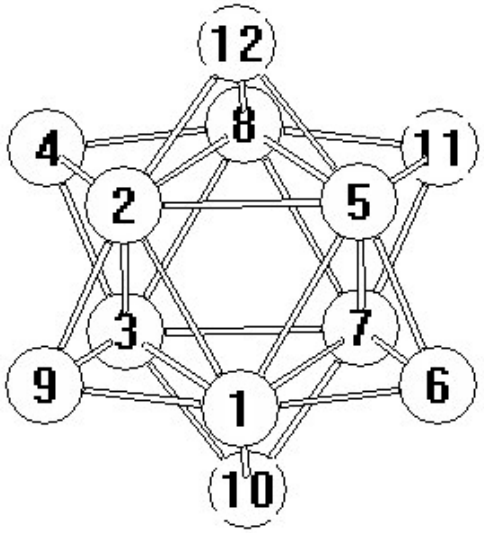
Charge 2+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.913779	0.000000			
3	Ge	2.861760	3.078752	0.000000		
4	Ge	4.517001	2.702173	2.487721	0.000000	
5	Ge	2.957017	2.939404	4.062196	4.462786	0.000000
6	Ge	2.476709	4.518942	4.462786	5.975700	2.487721
7	Ge	3.171888	4.442541	2.939404	4.518942	3.078752
8	Ge	4.167229	3.171888	2.957017	2.476709	2.861760
9	Ge	2.455564	2.432353	2.770301	3.707479	4.524112
10	Ge	2.719632	4.793049	2.476889	4.923573	4.603673
11	Ge	4.748109	4.882948	4.524112	4.899034	2.770301
12	Ge	4.512711	2.443939	4.603673	3.562441	2.476889

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.702173	0.000000			
8	Ge	4.517001	2.913779	0.000000		
9	Ge	4.899034	4.882948	4.748109	0.000000	
10	Ge	3.562441	2.443939	4.512711	3.933358	0.000000
11	Ge	3.707479	2.432353	2.455564	6.307367	4.847494
12	Ge	4.923573	4.793049	2.719632	4.847494	6.177065

		11	12
11	Ge	0.000000	
12	Ge	3.933358	0.000000



2-1.1 CubTetracap – $D_{4h}{}^{T}$ → C_i [22-1]

- 24899.7788256 (**+0.00 kcal/mol**)

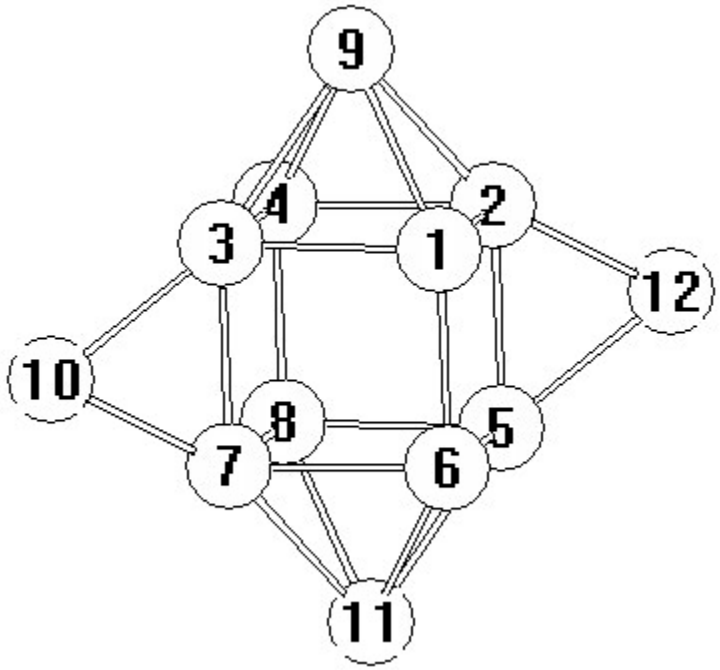
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.566528	0.000000			
3	Ge	2.565780	3.626034	0.000000		
4	Ge	3.631873	2.565108	2.567203	0.000000	
5	Ge	3.618988	2.570624	4.448065	3.617545	0.000000
6	Ge	2.526197	3.615015	3.617545	4.423691	2.567203
7	Ge	3.614441	4.441529	2.570624	3.615015	3.626034
8	Ge	4.424399	3.614441	3.618988	2.526197	2.565780
9	Ge	2.731692	2.711680	2.713877	2.730873	4.934634
10	Ge	4.663710	6.050795	2.624019	4.654347	6.053509
11	Ge	4.914123	4.932898	4.934634	4.914260	2.713877
12	Ge	4.655671	2.624744	6.053509	4.664695	2.624019

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.565108	0.000000			
8	Ge	3.631873	2.566528	0.000000		
9	Ge	4.914260	4.932898	4.914123	0.000000	
10	Ge	4.664695	2.624744	4.655671	5.267461	0.000000
11	Ge	2.730873	2.711680	2.731692	6.606527	5.264481
12	Ge	4.654347	6.050795	4.663710	5.264481	8.202172

		11	12
11	Ge	0.000000	
12	Ge	5.267461	0.000000



2-1.1 CubTetracap – D_{4h} → C_i [20-4(?)]

- 24898.5964116 (+13.02 kcal/mol)

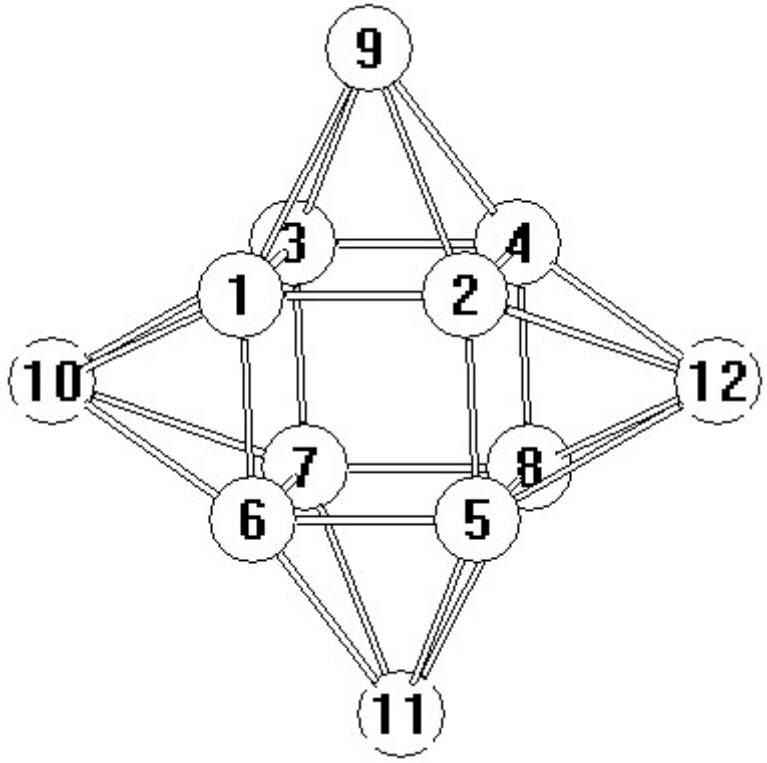
Charge 6+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.549524	0.000000			
3	Ge	2.703626	3.716136	0.000000		
4	Ge	3.716136	2.703626	2.549524	0.000000	
5	Ge	3.605571	2.549524	4.506633	3.716136	0.000000
6	Ge	2.549524	3.605571	3.716136	4.506633	2.549524
7	Ge	3.716136	4.506633	2.549524	3.605571	3.716136
8	Ge	4.506633	3.716136	3.605571	2.549524	2.703626
9	Ge	3.114989	3.114989	3.114989	3.114989	5.380670
10	Ge	3.114989	5.380670	3.114989	5.380670	5.380670
11	Ge	5.380670	5.380670	5.380670	5.380670	3.114989
12	Ge	5.380670	3.114989	5.380670	3.114989	3.114989

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.703626	0.000000			
8	Ge	3.716136	2.549524	0.000000		
9	Ge	5.380670	5.380670	5.380670	0.000000	
10	Ge	3.114989	3.114989	5.380670	5.338529	0.000000
11	Ge	3.114989	3.114989	3.114989	7.549821	5.338529
12	Ge	5.380670	5.380670	3.114989	5.338529	7.549821

		11	12
11	Ge	0.000000	
12	Ge	5.338529	0.000000



2-1 CubTetracap – D_{4h} [HE]

-24896.8900486 (+97.58 kcal/mol)

Ge_{12} – 2-2_CubTetracap-C_{2v}

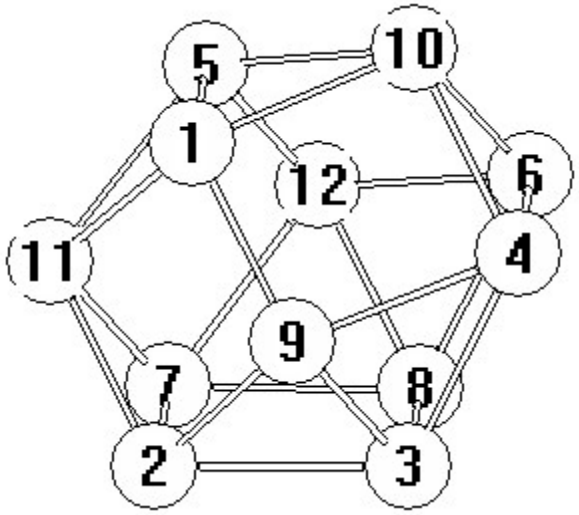
Charge 6-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.821401	0.000000			
3	Ge	4.454781	2.813038	0.000000		
4	Ge	3.821401	4.788279	2.813038	0.000000	
5	Ge	2.599522	4.630335	5.143528	4.630335	0.000000
6	Ge	4.630335	5.463042	3.821211	2.630059	3.821401
7	Ge	4.630335	2.630059	3.821211	5.463042	3.821401
8	Ge	5.143528	3.821211	2.543088	3.821211	4.454781
9	Ge	2.541452	2.813410	2.602069	2.813410	4.452782
10	Ge	2.814071	5.464080	4.630900	2.629816	2.814071
11	Ge	2.814071	2.629816	4.630900	5.464080	2.814071
12	Ge	4.452782	4.630400	4.455203	4.630400	2.541452

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.788279	0.000000			
8	Ge	2.813038	2.813038	0.000000		
9	Ge	4.630400	4.630400	4.455203	0.000000	
10	Ge	2.629816	5.464080	4.630900	3.820768	0.000000
11	Ge	5.464080	2.629816	4.630900	3.820768	4.790914
12	Ge	2.813410	2.813410	2.602069	5.142594	3.820768

		11	12
11	Ge	0.000000	
12	Ge	3.820768	0.000000



2-2 CubTetracap – C_{2v} [30-4]

- 24898.9354199 (+67.70 kcal/mol)

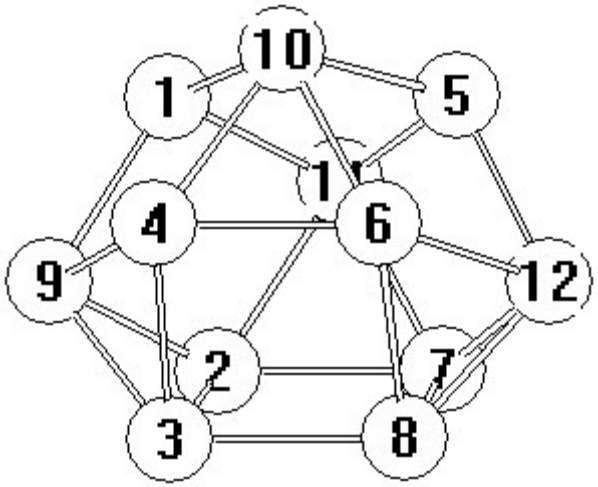
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.306984	0.000000			
3	Ge	4.220046	2.774732	0.000000		
4	Ge	3.306984	4.327368	2.774732	0.000000	
5	Ge	3.324805	4.414402	5.174915	4.414402	0.000000
6	Ge	4.414402	5.033922	3.826016	2.571820	3.306984
7	Ge	4.414402	2.571820	3.826016	5.033922	3.306984
8	Ge	5.174915	3.826016	2.698191	3.826016	4.220046
9	Ge	2.585522	2.692057	2.457777	2.692057	5.080543
10	Ge	2.579816	4.861566	4.627650	2.585758	2.579816
11	Ge	2.579816	2.585758	4.627650	4.861566	2.579816
12	Ge	5.080543	4.694931	4.643582	4.694931	2.585522

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.327368	0.000000			
8	Ge	2.774732	2.774732	0.000000		
9	Ge	4.694931	4.694931	4.643582	0.000000	
10	Ge	2.585758	4.861566	4.627650	4.035816	0.000000
11	Ge	4.861566	2.585758	4.627650	4.035816	3.916625
12	Ge	2.692057	2.692057	2.457777	5.752815	4.035816

		11	12
11	Ge	0.000000	
12	Ge	4.035816	0.000000



2-2 CubTetracap – C_{2v} [HE]

- 24899.9141039 (+27.66 kcal/mol)

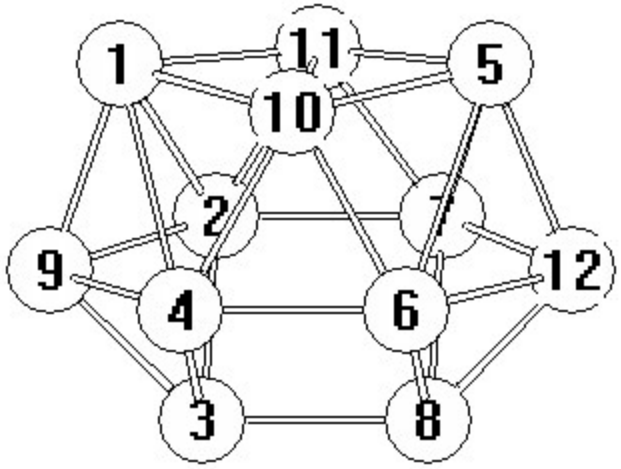
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.182173	0.000000			
3	Ge	4.254725	2.732126	0.000000		
4	Ge	3.182173	4.022229	2.732126	0.000000	
5	Ge	4.214789	4.582977	5.385684	4.582977	0.000000
6	Ge	4.582977	4.778993	3.760392	2.580784	3.182173
7	Ge	4.582977	2.580784	3.760392	4.778993	3.182173
8	Ge	5.385684	3.760392	2.586823	3.760392	4.254725
9	Ge	2.569979	2.635644	2.448037	2.635644	5.641272
10	Ge	2.521022	4.213249	4.424603	2.590153	2.521022
11	Ge	2.521022	2.590153	4.424603	4.213249	2.521022
12	Ge	5.641272	4.731672	4.633694	4.731672	2.569979

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.022229	0.000000			
8	Ge	2.732126	2.732126	0.000000		
9	Ge	4.731672	4.731672	4.633694	0.000000	
10	Ge	2.590153	4.213249	4.424603	3.981163	0.000000
11	Ge	4.213249	2.590153	4.424603	3.981163	2.745387
12	Ge	2.635644	2.635644	2.448037	5.983492	3.981163

		11	12
11	Ge	0.000000	
12	Ge	3.981163	0.000000



2-2 CubTetracap – C_{2v} [26-3]

- 24900.4118802 (+23.78 kcal/mol)

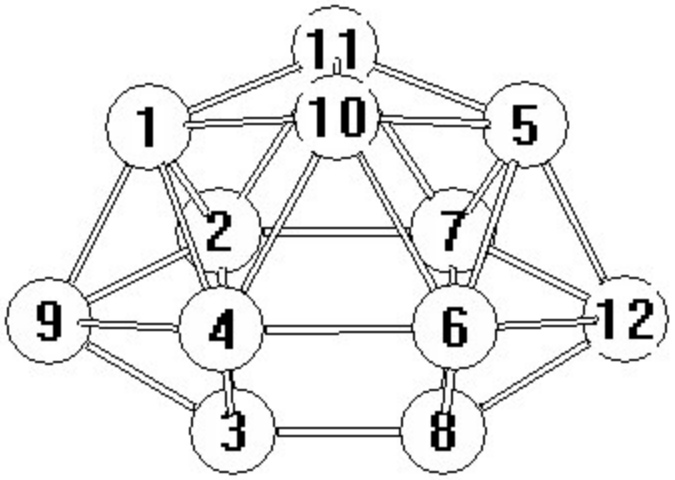
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.820296	0.000000			
3	Ge	3.637030	2.691808	0.000000		
4	Ge	2.820296	4.091699	2.691808	0.000000	
5	Ge	4.190536	4.346279	4.798830	4.346279	0.000000
6	Ge	4.346279	4.853100	3.653681	2.609707	2.820296
7	Ge	4.346279	2.609707	3.653681	4.853100	2.820296
8	Ge	4.798830	3.653681	2.338789	3.653681	3.637030
9	Ge	2.486074	2.822174	2.399572	2.822174	5.740496
10	Ge	2.567060	4.324822	4.405513	2.694135	2.567060
11	Ge	2.567060	2.694135	4.405513	4.324822	2.567060
12	Ge	5.740496	4.963639	4.549740	4.963639	2.486074

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.091699	0.000000			
8	Ge	2.691808	2.691808	0.000000		
9	Ge	4.963639	4.963639	4.549740	0.000000	
10	Ge	2.694135	4.324822	4.405513	4.424569	0.000000
11	Ge	4.324822	2.694135	4.405513	4.424569	2.797302
12	Ge	2.822174	2.822174	2.399572	6.388856	4.424569

		11	12
11	Ge	0.000000	
12	Ge	4.424569	0.000000



2-2 CubTetracap – C_{2v} [24-4]

- 24900.3409776 (+26.27 kcal/mol)

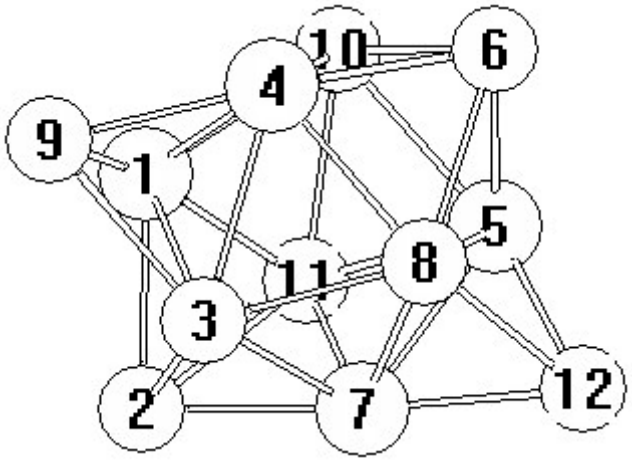
Charge 2+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.602309	0.000000			
3	Ge	3.007959	2.753918	0.000000		
4	Ge	2.607894	4.342451	2.745770	0.000000	
5	Ge	3.922811	4.391440	4.253073	3.598414	0.000000
6	Ge	4.391440	5.794640	4.485398	2.522703	2.602309
7	Ge	3.598414	2.522703	2.697571	3.940663	2.607894
8	Ge	4.253073	4.485398	2.541567	2.697571	3.007959
9	Ge	2.532816	3.905055	2.642757	2.560781	5.576494
10	Ge	2.606766	4.554608	4.516336	2.695822	2.657191
11	Ge	2.657191	2.764411	4.195650	4.162629	2.606766
12	Ge	5.576494	5.079054	4.401824	4.851254	2.532816

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.342451	0.000000			
8	Ge	2.753918	2.745770	0.000000		
9	Ge	5.079054	4.851254	4.401824	0.000000	
10	Ge	2.764411	4.162629	4.195650	4.409682	0.000000
11	Ge	4.554608	2.695822	4.516336	5.028911	2.753852
12	Ge	3.905055	2.560781	2.642757	6.592651	5.028911

		11	12
11	Ge	0.000000	
12	Ge	4.409682	0.000000



2-2.1 CubTetracap – C_{2v} → C_2 [22-2]

- 24899.7678549 (+6.88 kcal/mol)

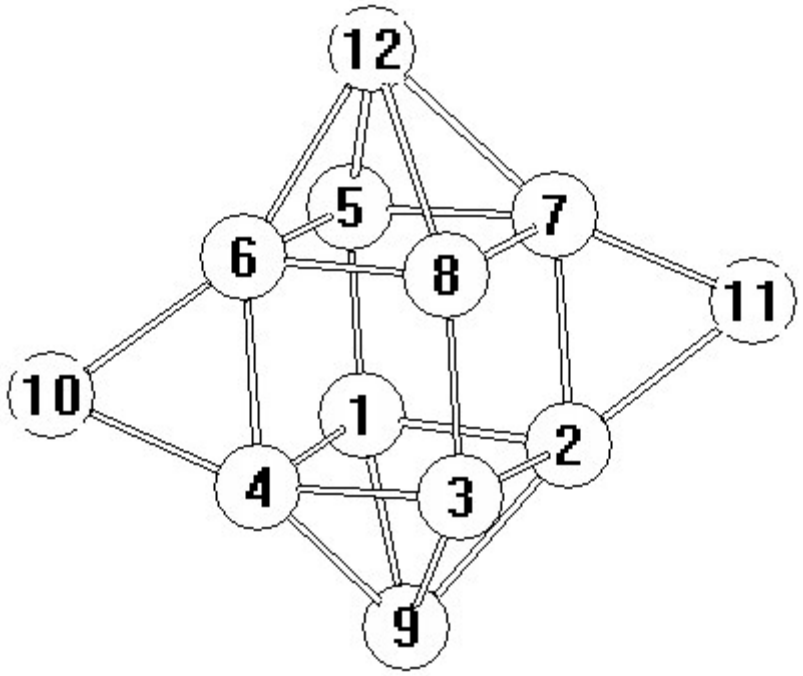
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.635626	0.000000			
3	Ge	3.644519	2.502544	0.000000		
4	Ge	2.635626	3.615663	2.502544	0.000000	
5	Ge	2.394829	3.642402	4.401386	3.642402	0.000000
6	Ge	3.642402	4.476458	3.601936	2.639254	2.635626
7	Ge	3.642402	2.639254	3.601936	4.476458	2.635626
8	Ge	4.401386	3.601936	2.542845	3.601936	3.644519
9	Ge	2.479796	2.777157	3.139928	2.777157	4.699488
10	Ge	4.607246	6.034370	4.662688	2.630203	4.607246
11	Ge	4.607246	2.630203	4.662688	6.034370	4.607246
12	Ge	4.699488	5.027410	5.174927	5.027410	2.479796

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	3.615663	0.000000			
8	Ge	2.502544	2.502544	0.000000		
9	Ge	5.027410	5.027410	5.174927	0.000000	
10	Ge	2.630203	6.034370	4.662688	5.288016	0.000000
11	Ge	6.034370	2.630203	4.662688	5.288016	8.157746
12	Ge	2.777157	2.777157	3.139928	6.654250	5.288016

		11	12
11	Ge	0.000000	
12	Ge	5.288016	0.000000



2-2 CubTetracap – C_{2v} [20-4]

- 24898.6005071 (+10.45 kcal/mol)

Ge_{12} – 3-1_PrHex-D_{6h}

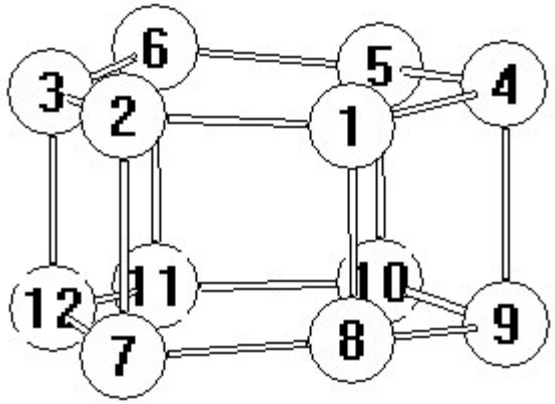
Charge 6-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.544963	0.000000			
3	Ge	4.028103	2.545029	0.000000		
4	Ge	2.544963	4.698807	5.039982	0.000000	
5	Ge	4.028103	5.039982	4.027458	2.545029	0.000000
6	Ge	5.040576	4.699004	2.544770	4.699004	2.544770
7	Ge	3.608045	2.693560	3.608111	5.416091	5.651788
8	Ge	2.428442	3.608045	4.703516	3.608045	4.703516
9	Ge	3.608045	5.416091	5.651788	2.693560	3.608111
10	Ge	4.703516	5.651788	4.702977	3.608111	2.428492
11	Ge	5.652406	5.416379	3.608085	5.416379	3.608085
12	Ge	4.703516	3.608111	2.428492	5.651788	4.702977

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	5.416379	0.000000			
8	Ge	5.652406	2.544963	0.000000		
9	Ge	5.416379	4.698807	2.544963	0.000000	
10	Ge	3.608085	5.039982	4.028103	2.545029	0.000000
11	Ge	2.694027	4.699004	5.040576	4.699004	2.544770
12	Ge	3.608085	2.545029	4.028103	5.039982	4.027458

		11	12
11	Ge	0.000000	
12	Ge	2.544770	0.000000



3-1.1 PrHex – D_{6h} → C_{2v} [30-2]

- 24898.9688886 (+46.70 kcal/mol)

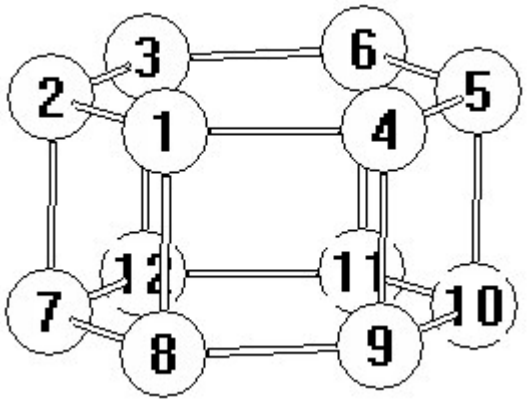
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.450140	0.000000			
3	Ge	4.426416	2.547843	0.000000		
4	Ge	2.450140	4.029955	4.767547	0.000000	
5	Ge	4.426416	4.767547	4.029325	2.547843	0.000000
6	Ge	5.334822	4.426931	2.450123	4.426931	2.450123
7	Ge	3.479424	2.428128	3.519469	4.704927	5.350202
8	Ge	2.513543	3.479424	5.069091	3.479424	5.069091
9	Ge	3.479424	4.704927	5.350202	2.428128	3.519469
10	Ge	5.069091	5.350202	4.704249	3.519469	2.427860
11	Ge	5.897348	5.069655	3.479383	5.069655	3.479383
12	Ge	5.069091	3.519469	2.427860	5.350202	4.704249

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	5.069655	0.000000			
8	Ge	5.897348	2.450140	0.000000		
9	Ge	5.069655	4.029955	2.450140	0.000000	
10	Ge	3.479383	4.767547	4.426416	2.547843	0.000000
11	Ge	2.513738	4.426931	5.334822	4.426931	2.450123
12	Ge	3.479383	2.547843	4.426416	4.767547	4.029325

		11	12
11	Ge	0.000000	
12	Ge	2.450123	0.000000



3-1.1 PrHex – D_{6h} [T] → C_{2v} [HE]

- 24899.9096134 (+30.47 kcal/mol)

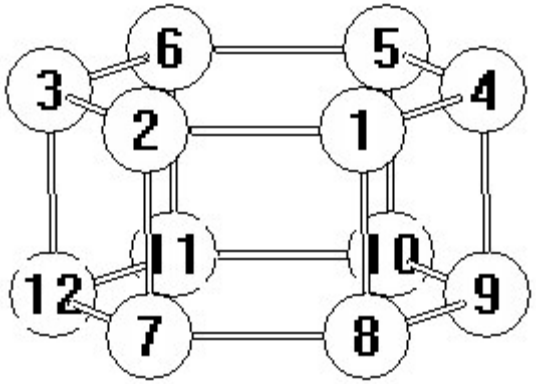
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.464784	0.000000			
3	Ge	4.269131	2.464784	0.000000		
4	Ge	2.464784	4.269131	4.929567	0.000000	
5	Ge	4.269131	4.929567	4.269131	2.464784	0.000000
6	Ge	4.929567	4.269131	2.464784	4.269131	2.464784
7	Ge	3.435972	2.393898	3.435972	4.894510	5.480090
8	Ge	2.393898	3.435972	4.894510	3.435972	4.894510
9	Ge	3.435972	4.894510	5.480090	2.393898	3.435972
10	Ge	4.894510	5.480090	4.894510	3.435972	2.393898
11	Ge	5.480090	4.894510	3.435972	4.894510	3.435972
12	Ge	4.894510	3.435972	2.393898	5.480090	4.894510

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.894510	0.000000			
8	Ge	5.480090	2.464784	0.000000		
9	Ge	4.894510	4.269131	2.464784	0.000000	
10	Ge	3.435972	4.929567	4.269131	2.464784	0.000000
11	Ge	2.393898	4.269131	4.929567	4.269131	2.464784
12	Ge	3.435972	2.464784	4.269131	4.929567	4.269131

		11	12
11	Ge	0.000000	
12	Ge	2.464784	0.000000



3-1 PrHex – D_{6h} [HE]

- 24900.3835985 (+41.53 kcal/mol)

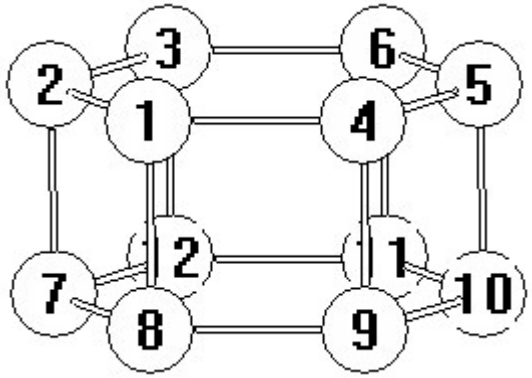
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.435566	0.000000			
3	Ge	4.218523	2.435566	0.000000		
4	Ge	2.435566	4.218523	4.871131	0.000000	
5	Ge	4.218523	4.871131	4.218523	2.435566	0.000000
6	Ge	4.871131	4.218523	2.435566	4.218523	2.435566
7	Ge	3.424132	2.406803	3.424132	4.856814	5.433288
8	Ge	2.406803	3.424132	4.856814	3.424132	4.856814
9	Ge	3.424132	4.856814	5.433288	2.406803	3.424132
10	Ge	4.856814	5.433288	4.856814	3.424132	2.406803
11	Ge	5.433288	4.856814	3.424132	4.856814	3.424132
12	Ge	4.856814	3.424132	2.406803	5.433288	4.856814

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.856814	0.000000			
8	Ge	5.433288	2.435566	0.000000		
9	Ge	4.856814	4.218523	2.435566	0.000000	
10	Ge	3.424132	4.871131	4.218523	2.435566	0.000000
11	Ge	2.406803	4.218523	4.871131	4.218523	2.435566
12	Ge	3.424132	2.435566	4.218523	4.871131	4.218523

		11	12
11	Ge	0.000000	
12	Ge	2.435566	0.000000



3-1 PrHex – D_{6h} [T] [HE]

- 24900.3300045 (+33.15 kcal/mol)

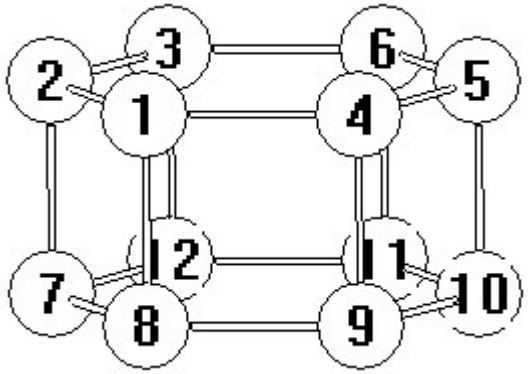
Charge 2+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.428581	0.000000			
3	Ge	4.206425	2.428581	0.000000		
4	Ge	2.428581	4.206425	4.857162	0.000000	
5	Ge	4.206425	4.857162	4.206425	2.428581	0.000000
6	Ge	4.857162	4.206425	2.428581	4.206425	2.428581
7	Ge	3.435796	2.430368	3.435796	4.858055	5.431271
8	Ge	2.430368	3.435796	4.858055	3.435796	4.858055
9	Ge	3.435796	4.858055	5.431271	2.430368	3.435796
10	Ge	4.858055	5.431271	4.858055	3.435796	2.430368
11	Ge	5.431271	4.858055	3.435796	4.858055	3.435796
12	Ge	4.858055	3.435796	2.430368	5.431271	4.858055

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.858055	0.000000			
8	Ge	5.431271	2.428581	0.000000		
9	Ge	4.858055	4.206425	2.428581	0.000000	
10	Ge	3.435796	4.857162	4.206425	2.428581	0.000000
11	Ge	2.430368	4.206425	4.857162	4.206425	2.428581
12	Ge	3.435796	2.428581	4.206425	4.857162	4.206425

		11	12
11	Ge	0.000000	
12	Ge	2.428581	0.000000



3-1 PrHex – D_{6h} [HE]

- 24899.7409047 (+23.80 kcal/mol)

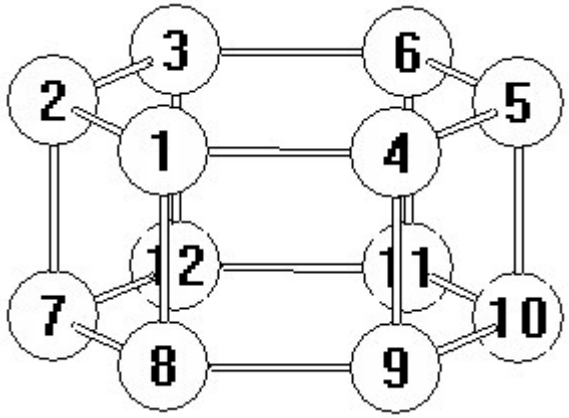
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.524373	0.000000			
3	Ge	4.372342	2.524373	0.000000		
4	Ge	2.524373	4.372342	5.048745	0.000000	
5	Ge	4.372342	5.048745	4.372342	2.524373	0.000000
6	Ge	5.048745	4.372342	2.524373	4.372342	2.524373
7	Ge	3.488892	2.408300	3.488892	4.991721	5.593723
8	Ge	2.408300	3.488892	4.991721	3.488892	4.991721
9	Ge	3.488892	4.991721	5.593723	2.408300	3.488892
10	Ge	4.991721	5.593723	4.991721	3.488892	2.408300
11	Ge	5.593723	4.991721	3.488892	4.991721	3.488892
12	Ge	4.991721	3.488892	2.408300	5.593723	4.991721

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.991721	0.000000			
8	Ge	5.593723	2.524373	0.000000		
9	Ge	4.991721	4.372342	2.524373	0.000000	
10	Ge	3.488892	5.048745	4.372342	2.524373	0.000000
11	Ge	2.408300	4.372342	5.048745	4.372342	2.524373
12	Ge	3.488892	2.524373	4.372342	5.048745	4.372342

		11	12
11	Ge	0.000000	
12	Ge	2.524373	0.000000



3-1 Prhex – D_{6h} [20-5]

- 24898.5957133 (+13.46 kcal/mol)

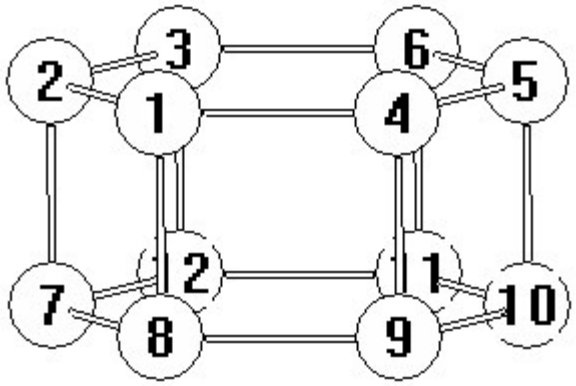
Charge 6+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.644819	0.000000			
3	Ge	4.580960	2.644819	0.000000		
4	Ge	2.644819	4.580960	5.289637	0.000000	
5	Ge	4.580960	5.289637	4.580960	2.644819	0.000000
6	Ge	5.289637	4.580960	2.644819	4.580960	2.644819
7	Ge	3.661016	2.531398	3.661016	5.233848	5.864148
8	Ge	2.531398	3.661016	5.233848	3.661016	5.233848
9	Ge	3.661016	5.233848	5.864148	2.531398	3.661016
10	Ge	5.233848	5.864148	5.233848	3.661016	2.531398
11	Ge	5.864148	5.233848	3.661016	5.233848	3.661016
12	Ge	5.233848	3.661016	2.531398	5.864148	5.233848

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	5.233848	0.000000			
8	Ge	5.864148	2.644819	0.000000		
9	Ge	5.233848	4.580960	2.644819	0.000000	
10	Ge	3.661016	5.289637	4.580960	2.644819	0.000000
11	Ge	2.531398	4.580960	5.289637	4.580960	2.644819
12	Ge	3.661016	2.644819	4.580960	5.289637	4.580960

		11	12
11	Ge	0.000000	
12	Ge	2.644819	0.000000



3-1 Prhex – D_{6h} [T] [HE]

- 24896.8667439 (+112.21 kcal/mol)

Ge_{12} – 3-2_AntiPrHex-D_{6d}

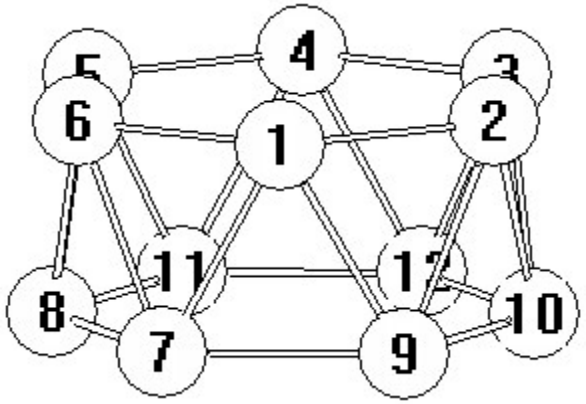
Charge 6-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.623070	0.000000			
3	Ge	4.543290	2.623070	0.000000		
4	Ge	5.246140	4.543290	2.623070	0.000000	
5	Ge	4.543290	5.246140	4.543290	2.623070	0.000000
6	Ge	2.623070	4.543290	5.246140	4.543290	2.623070
7	Ge	2.728004	4.399929	5.592561	5.592561	4.399929
8	Ge	4.399929	5.592561	5.592561	4.399929	2.728004
9	Ge	2.728004	2.728004	4.399929	5.592561	5.592561
10	Ge	4.399929	2.728004	2.728004	4.399929	5.592561
11	Ge	5.592561	5.592561	4.399929	2.728004	2.728004
12	Ge	5.592561	4.399929	2.728004	2.728004	4.399929

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.728004	0.000000			
8	Ge	2.728004	2.623070	0.000000		
9	Ge	4.399929	2.623070	4.543290	0.000000	
10	Ge	5.592561	4.543290	5.246140	2.623070	0.000000
11	Ge	4.399929	4.543290	2.623070	5.246140	4.543290
12	Ge	5.592561	5.246140	4.543290	4.543290	2.623070

		11	12
11	Ge	0.000000	
12	Ge	2.623070	0.000000



3-2 AntiPrHex – D_{6d} [30-5]

- 24898.9321164 (+69.78 kcal/mol)

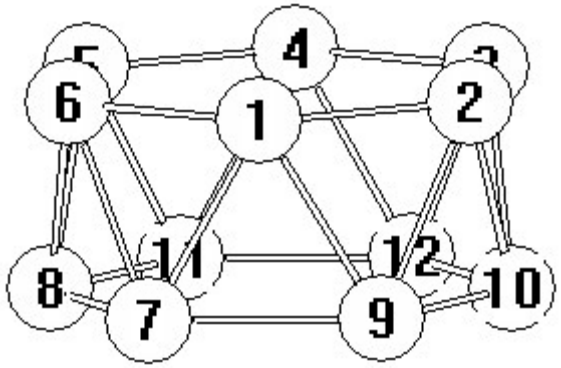
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.569471	0.000000			
3	Ge	4.450454	2.569471	0.000000		
4	Ge	5.138942	4.450454	2.569471	0.000000	
5	Ge	4.450454	5.138942	4.450454	2.569471	0.000000
6	Ge	2.569471	4.450454	5.138942	4.450454	2.569471
7	Ge	2.653014	4.298115	5.468922	5.468922	4.298115
8	Ge	4.298115	5.468922	5.468922	4.298115	2.653014
9	Ge	2.653014	2.653014	4.298115	5.468922	5.468922
10	Ge	4.298115	2.653014	2.653014	4.298115	5.468922
11	Ge	5.468922	5.468922	4.298115	2.653014	2.653014
12	Ge	5.468922	4.298115	2.653014	2.653014	4.298115

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.653014	0.000000			
8	Ge	2.653014	2.569471	0.000000		
9	Ge	4.298115	2.569471	4.450454	0.000000	
10	Ge	5.468922	4.450454	5.138942	2.569471	0.000000
11	Ge	4.298115	4.450454	2.569471	5.138942	4.450454
12	Ge	5.468922	5.138942	4.450454	4.450454	2.569471

		11	12
11	Ge	0.000000	
12	Ge	2.569471	0.000000



3-2 AntiPrHex – D_{6d} [T] [HE]

- 24899.8789618 (+49.71 kcal/mol)

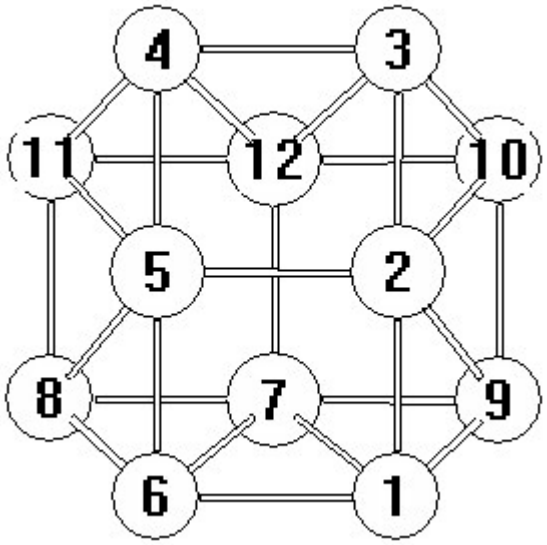
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.495214	0.000000			
3	Ge	4.973714	2.496098	0.000000		
4	Ge	5.643247	3.652159	2.671440	0.000000	
5	Ge	3.652159	2.666021	3.655484	2.495214	0.000000
6	Ge	2.671440	3.655484	5.648238	4.973714	2.496098
7	Ge	2.792917	3.032140	4.590394	4.588921	3.032140
8	Ge	4.444334	4.588921	5.748970	4.444334	2.792917
9	Ge	2.544940	2.794546	4.446940	5.748970	4.590394
10	Ge	4.444334	2.792917	2.544940	4.444334	4.588921
11	Ge	5.748970	4.590394	4.446940	2.544940	2.794546
12	Ge	4.588921	3.032140	2.794546	2.792917	3.032140

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.794546	0.000000			
8	Ge	2.544940	2.495214	0.000000		
9	Ge	4.446940	2.496098	4.973714	0.000000	
10	Ge	5.748970	3.652159	5.643247	2.671440	0.000000
11	Ge	4.446940	3.655484	2.671440	5.648238	4.973714
12	Ge	4.590394	2.666021	3.652159	3.655484	2.495214

		11	12
11	Ge	0.000000	
12	Ge	2.496098	0.000000



3-2.1 AntiPrHex – D_{6d} → S_4 [24-3]

- 24900.3459408 (+23.15 kcal/mol)

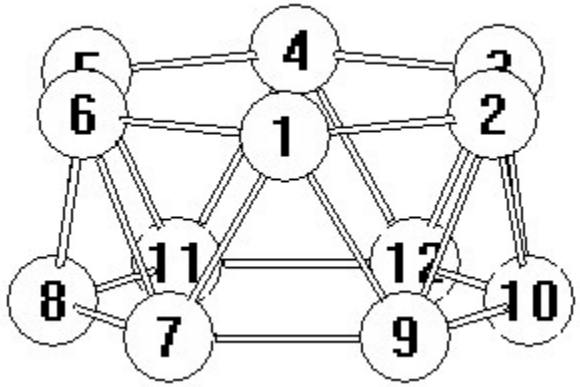
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.582871	0.000000			
3	Ge	4.473664	2.582871	0.000000		
4	Ge	5.165742	4.473664	2.582871	0.000000	
5	Ge	4.473664	5.165742	4.473664	2.582871	0.000000
6	Ge	2.582871	4.473664	5.165742	4.473664	2.582871
7	Ge	2.647547	4.308642	5.488105	5.488105	4.308642
8	Ge	4.308642	5.488105	5.488105	4.308642	2.647547
9	Ge	2.647547	2.647547	4.308642	5.488105	5.488105
10	Ge	4.308642	2.647547	2.647547	4.308642	5.488105
11	Ge	5.488105	5.488105	4.308642	2.647547	2.647547
12	Ge	5.488105	4.308642	2.647547	2.647547	4.308642

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.647547	0.000000			
8	Ge	2.647547	2.582871	0.000000		
9	Ge	4.308642	2.582871	4.473664	0.000000	
10	Ge	5.488105	4.473664	5.165742	2.582871	0.000000
11	Ge	4.308642	4.473664	2.582871	5.165742	4.473664
12	Ge	5.488105	5.165742	4.473664	4.473664	2.582871

		11	12
11	Ge	0.000000	
12	Ge	2.582871	0.000000



3-2 AntiPrHex – D_{6d} [HE]

- 24898.5100093 (+67.24 kcal/mol)

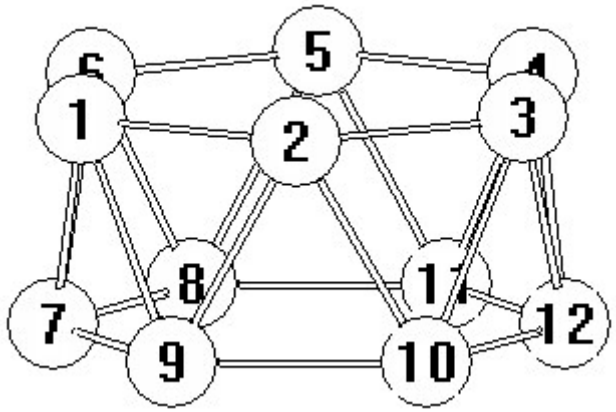
Charge
6+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.705528	0.000000			
3	Ge	4.686112	2.705528	0.000000		
4	Ge	5.411056	4.686112	2.705528	0.000000	
5	Ge	4.686112	5.411056	4.686112	2.705528	0.000000
6	Ge	2.705528	4.686112	5.411056	4.686112	2.705528
7	Ge	2.828565	4.547437	5.775603	5.775603	4.547437
8	Ge	4.547437	5.775603	5.775603	4.547437	2.828565
9	Ge	2.828565	2.828565	4.547437	5.775603	5.775603
10	Ge	4.547437	2.828565	2.828565	4.547437	5.775603
11	Ge	5.775603	5.775603	4.547437	2.828565	2.828565
12	Ge	5.775603	4.547437	2.828565	2.828565	4.547437

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.828565	0.000000			
8	Ge	2.828565	2.705528	0.000000		
9	Ge	4.547437	2.705528	4.686112	0.000000	
10	Ge	5.775603	4.686112	5.411056	2.705528	0.000000
11	Ge	4.547437	4.686112	2.705528	5.411056	4.686112
12	Ge	5.775603	5.411056	4.686112	4.686112	2.705528

		11	12
11	Ge	0.000000	
12	Ge	2.705528	0.000000



3-2 AntiPrHex – D_{6d} [HE]

- 24896.7855334 (+163.17 kcal/mol)

Ge_{12} – 4-1_Icosaedru-I_h

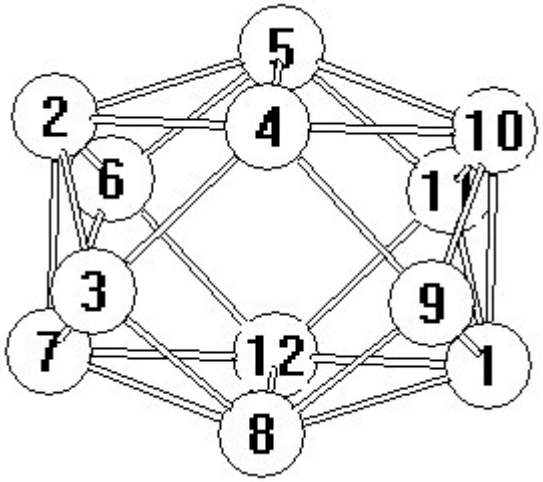
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	5.576355	0.000000			
3	Ge	4.972478	2.535769	0.000000		
4	Ge	4.227793	2.857594	2.671060	0.000000	
5	Ge	4.227901	2.857433	4.353200	2.854078	0.000000
6	Ge	4.972746	2.535683	4.140196	4.353403	2.671146
7	Ge	4.871399	2.708030	2.536593	4.225295	4.225186
8	Ge	2.857433	4.227901	2.673884	3.583107	4.580875
9	Ge	2.535683	4.972746	3.751879	2.673971	4.355137
10	Ge	2.708030	4.871400	4.968861	2.855729	2.855890
11	Ge	2.535768	4.972477	5.587091	4.354933	2.673883
12	Ge	2.857594	4.227793	4.354933	4.580875	3.583107

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.536507	0.000000			
8	Ge	4.355137	2.855890	0.000000		
9	Ge	5.587491	4.969130	2.671146	0.000000	
10	Ge	4.969130	5.570655	4.225186	2.536507	0.000000
11	Ge	3.751879	4.968861	4.353199	4.140196	2.536593
12	Ge	2.673971	2.855729	2.854078	4.353403	4.225295

		11	12
11	Ge	0.000000	
12	Ge	2.671059	0.000000



4-1 Icosaedru – I_h (C_1) [28-3]

- 24899.9406208 (+11.02 kcal/mol)

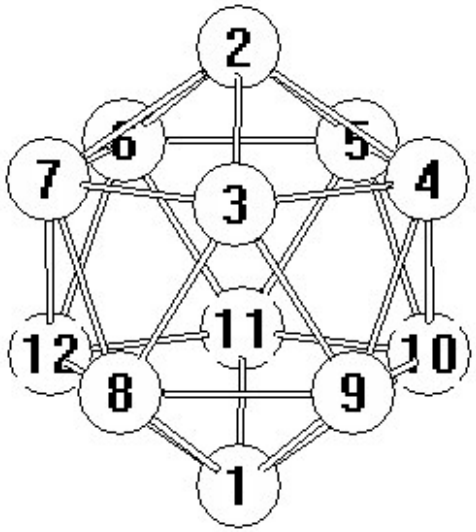
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	5.110041	0.000000			
3	Ge	4.346820	2.686555	0.000000		
4	Ge	4.347068	2.686292	2.686285	0.000000	
5	Ge	4.347068	2.686292	4.346781	2.686539	0.000000
6	Ge	4.346820	2.686555	4.346997	4.346781	2.686285
7	Ge	4.346089	2.685838	2.686077	4.345840	4.345840
8	Ge	2.686293	4.347068	2.686738	4.346989	5.110167
9	Ge	2.686555	4.346820	2.686250	2.686738	4.347061
10	Ge	2.685838	4.346089	4.345930	2.686361	2.686361
11	Ge	2.686555	4.346820	5.110022	4.347061	2.686738
12	Ge	2.686292	4.347068	4.347061	5.110167	4.346989

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.686077	0.000000			
8	Ge	4.347061	2.686361	0.000000		
9	Ge	5.110022	4.345930	2.686285	0.000000	
10	Ge	4.345930	5.108024	4.345840	2.686077	0.000000
11	Ge	2.686250	4.345930	4.346781	4.346997	2.686077
12	Ge	2.686738	2.686361	2.686539	4.346781	4.345840

		11	12
11	Ge	0.000000	
12	Ge	2.686285	0.000000



4-1 Icosaedru – I_h (C_1) [26-2]

- 24900.4408414 (+5.61 kcal/mol)

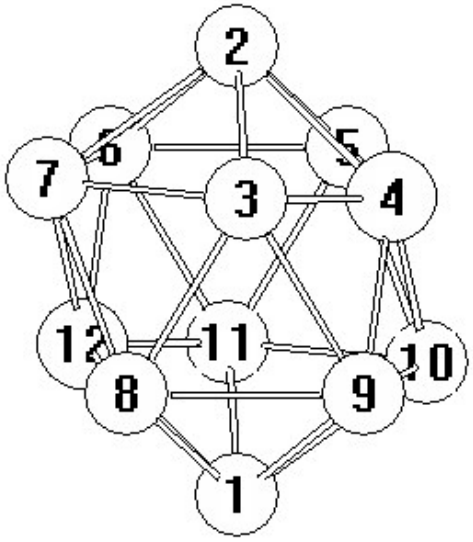
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	5.257067	0.000000			
3	Ge	4.459852	2.772385	0.000000		
4	Ge	3.994447	2.525068	2.519647	0.000000	
5	Ge	4.463661	2.767300	4.477553	2.524920	0.000000
6	Ge	4.481216	2.737335	4.457392	3.990114	2.733574
7	Ge	4.483243	2.745291	2.737210	3.994215	4.463476
8	Ge	2.767300	4.463661	2.733747	3.987708	5.246682
9	Ge	2.737334	4.481215	2.765066	2.519545	4.477423
10	Ge	2.745290	4.483242	4.481451	2.525303	2.767476
11	Ge	2.772385	4.459852	5.245573	3.990313	2.733746
12	Ge	2.525068	3.994446	3.990311	4.126304	3.987706

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.772301	0.000000			
8	Ge	4.477424	2.767476	0.000000		
9	Ge	5.245172	4.459592	2.733575	0.000000	
10	Ge	4.459592	5.256939	4.463476	2.772301	0.000000
11	Ge	2.765067	4.481451	4.477554	4.457392	2.737209
12	Ge	2.519544	2.525303	2.524920	3.990112	3.994212

		11	12
11	Ge	0.000000	
12	Ge	2.519646	0.000000



4-1.1 Icosaedru – I_h (C_1) → C_1 [24-2]

- 24900.3479326 (+21.90 kcal/mol)

Ge_{12} – 5-1_Td-4vf-S_4

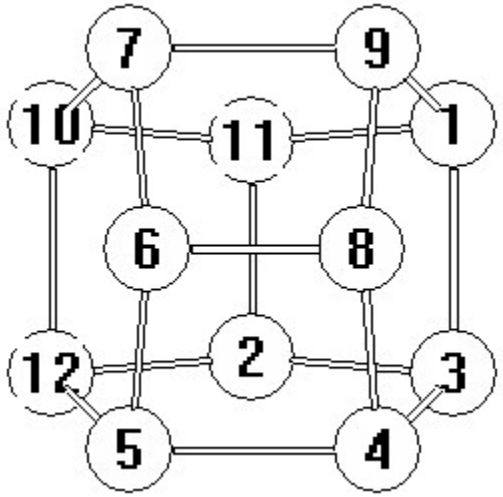
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.596594	0.000000			
3	Ge	2.814498	2.461830	0.000000		
4	Ge	4.333769	3.485726	2.437339	0.000000	
5	Ge	5.623253	3.485548	4.333595	2.814498	0.000000
6	Ge	4.826878	4.279242	4.826644	3.596594	2.461830
7	Ge	4.333769	4.826878	5.623253	5.360181	4.562154
8	Ge	3.485726	4.279242	3.485548	2.461753	3.597251
9	Ge	2.437339	4.826644	4.333595	4.562154	5.360762
10	Ge	4.562154	3.597251	5.360762	5.623253	4.333595
11	Ge	2.461753	2.443573	3.597251	4.826878	4.826644
12	Ge	5.360181	2.461753	4.562154	4.333769	2.437339

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.461753	0.000000			
8	Ge	2.443573	3.596594	0.000000		
9	Ge	3.597251	2.814498	2.461830	0.000000	
10	Ge	3.485548	2.437339	4.826644	4.333595	0.000000
11	Ge	4.279242	3.485726	4.279242	3.485548	2.461830
12	Ge	3.485726	4.333769	4.826878	5.623253	2.814498

		11	12
11	Ge	0.000000	
12	Ge	3.596594	0.000000



5-1 Td-4vf – S_4 [28-2]

- 24899.9514204 (+4.24 kcal/mol)

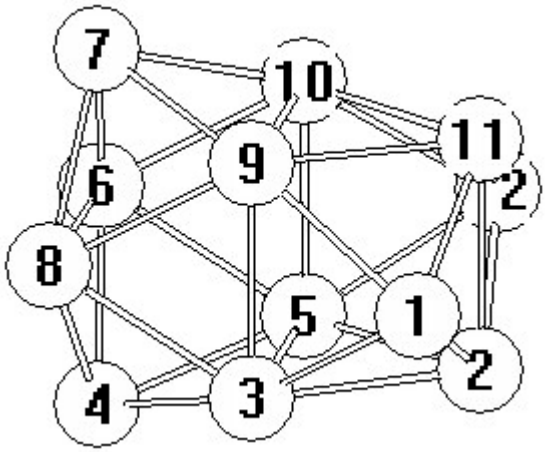
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.565098	0.000000			
3	Ge	2.621185	2.745030	0.000000		
4	Ge	5.157396	4.504402	2.622950	0.000000	
5	Ge	4.354018	2.742252	2.817935	2.621185	0.000000
6	Ge	5.669465	5.096934	3.912262	2.565098	2.745030
7	Ge	5.157396	5.669465	4.354018	4.292597	4.357234
8	Ge	4.504402	5.096934	2.742252	2.567273	3.913021
9	Ge	2.622950	3.912262	2.817935	4.357234	3.985160
10	Ge	4.357234	3.913021	3.985160	4.354018	2.817935
11	Ge	2.567273	2.761313	3.913021	5.669465	3.912262
12	Ge	4.292597	2.567273	4.357234	5.157396	2.622950

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.567273	0.000000			
8	Ge	2.761313	2.565098	0.000000		
9	Ge	3.913021	2.621185	2.745030	0.000000	
10	Ge	2.742252	2.622950	3.912262	2.817935	0.000000
11	Ge	5.096934	4.504402	5.096934	2.742252	2.745030
12	Ge	4.504402	5.157396	5.669465	4.354018	2.621185

		11	12
11	Ge	0.000000	
12	Ge	2.565098	0.000000



5-1 Td-4vf – S_4 [26-4]

- 24900.4064567 (+27.19 kcal/mol)

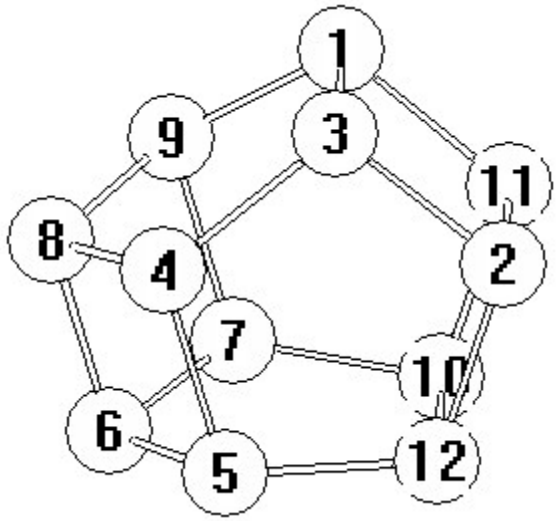
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.441759	0.000000			
3	Ge	2.505402	2.433777	0.000000		
4	Ge	4.020108	3.869469	2.459234	0.000000	
5	Ge	5.126738	3.870182	4.021196	2.505402	0.000000
6	Ge	4.950904	5.196923	4.951839	3.441759	2.433777
7	Ge	4.020108	4.950904	5.126738	4.752551	4.038397
8	Ge	3.869469	5.196923	3.870182	2.433783	3.440735
9	Ge	2.459234	4.951839	4.021196	4.038397	4.752329
10	Ge	4.038397	3.440735	4.752329	5.126738	4.021196
11	Ge	2.433783	2.362454	3.440735	4.950904	4.951839
12	Ge	4.752551	2.433783	4.038397	4.020108	2.459234

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.433783	0.000000			
8	Ge	2.362454	3.441759	0.000000		
9	Ge	3.440735	2.505402	2.433777	0.000000	
10	Ge	3.870182	2.459234	4.951839	4.021196	0.000000
11	Ge	5.196923	3.869469	5.196923	3.870182	2.433777
12	Ge	3.869469	4.020108	4.950904	5.126738	2.505402

		11	12
11	Ge	0.000000	
12	Ge	3.441759	0.000000



5-1 Td-4vf – S_4 [24-5]

- 24900.3394212 (+27.24 kcal/mol)

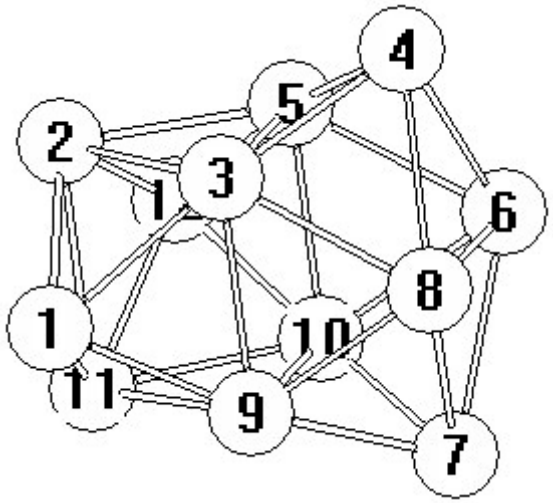
Charge 2+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.791627	0.000000			
3	Ge	2.499379	2.653696	0.000000		
4	Ge	4.974401	4.228833	2.500135	0.000000	
5	Ge	4.364564	2.653254	2.712722	2.499379	0.000000
6	Ge	5.597740	4.985048	3.844855	2.791627	2.653696
7	Ge	4.974401	5.597740	4.364564	4.717672	4.363899
8	Ge	4.228833	4.985048	2.653254	2.788860	3.843009
9	Ge	2.500135	3.844855	2.712722	4.363899	3.836368
10	Ge	4.363899	3.843009	3.836368	4.364564	2.712722
11	Ge	2.788860	2.851337	3.843009	5.597740	3.844855
12	Ge	4.717672	2.788860	4.363899	4.974401	2.500135

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.788860	0.000000			
8	Ge	2.851337	2.791627	0.000000		
9	Ge	3.843009	2.499379	2.653696	0.000000	
10	Ge	2.653254	2.500135	3.844855	2.712722	0.000000
11	Ge	4.985048	4.228833	4.985048	2.653254	2.653696
12	Ge	4.228833	4.974401	5.597740	4.364564	2.499379

		11	12
11	Ge	0.000000	
12	Ge	2.791627	0.000000



5-1 Td-4vf – S_4 [HE]

- 24899.7406806 (+23.94 kcal/mol)

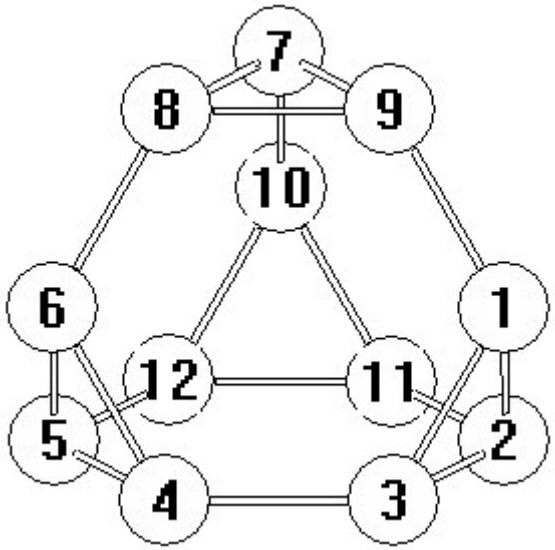
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.411607	0.000000			
3	Ge	2.411517	2.411047	0.000000		
4	Ge	4.229122	4.227702	2.472392	0.000000	
5	Ge	5.447578	4.883584	4.231237	2.411517	0.000000
6	Ge	4.880366	5.442449	4.228256	2.411607	2.411047
7	Ge	4.229122	4.880366	5.447578	5.448416	4.885597
8	Ge	4.227702	5.442449	4.883584	4.230010	4.228084
9	Ge	2.472392	4.228256	4.231237	4.885597	5.448273
10	Ge	4.885597	4.228084	5.448273	5.447578	4.231237
11	Ge	4.230010	2.470598	4.228084	4.880366	4.228256
12	Ge	5.448416	4.230010	4.885597	4.229122	2.472392

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.230010	0.000000			
8	Ge	2.470598	2.411607	0.000000		
9	Ge	4.228084	2.411517	2.411047	0.000000	
10	Ge	4.883584	2.472392	4.228256	4.231237	0.000000
11	Ge	5.442449	4.227702	5.442449	4.883584	2.411047
12	Ge	4.227702	4.229122	4.880366	5.447578	2.411517

		11	12
11	Ge	0.000000	
12	Ge	2.411607	0.000000



5-1 Td-4vf – S_4 [HE]

- 24898.3789197 (+149.50 kcal/mol)

Ge_{12} – 6-1_Cuboh-O_h

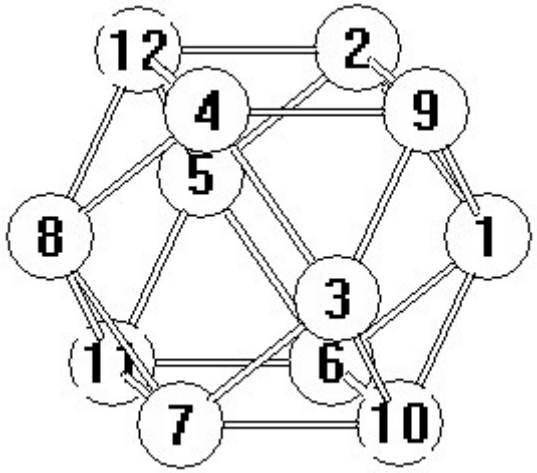
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.604928	0.000000			
3	Ge	3.683925	4.511868	0.000000		
4	Ge	4.511868	3.683925	2.604928	0.000000	
5	Ge	3.683925	2.604928	5.209856	4.511868	0.000000
6	Ge	2.604928	3.683925	4.511868	5.209856	2.604928
7	Ge	4.511868	5.209856	2.604928	3.683925	4.511868
8	Ge	5.209856	4.511868	3.683925	2.604928	3.683925
9	Ge	2.604928	2.604928	2.604928	2.604928	4.511868
10	Ge	2.604928	4.511868	2.604928	4.511868	4.511868
11	Ge	4.511868	4.511868	4.511868	4.511868	2.604928
12	Ge	4.511868	2.604928	4.511868	2.604928	2.604928

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	3.683925	0.000000			
8	Ge	4.511868	2.604928	0.000000		
9	Ge	4.511868	4.511868	4.511868	0.000000	
10	Ge	2.604928	2.604928	4.511868	3.683925	0.000000
11	Ge	2.604928	2.604928	2.604928	5.209856	3.683925
12	Ge	4.511868	4.511868	2.604928	3.683925	5.209856

		11	12
11	Ge	0.000000	
12	Ge	3.683925	0.000000



6-1 Cuboh – O_h [HE]

- 24900.3671486 (+51.85 kcal/mol)

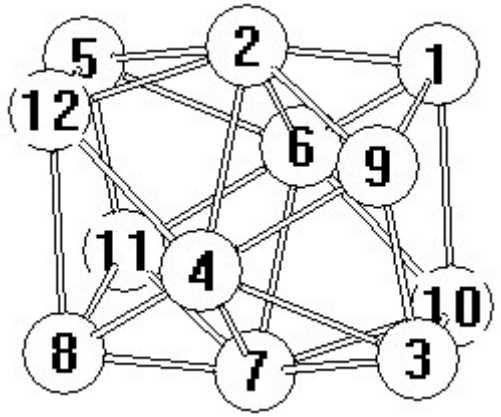
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.425412	0.000000			
3	Ge	3.740979	4.151246	0.000000		
4	Ge	4.177894	2.861546	2.750159	0.000000	
5	Ge	4.212218	2.751123	5.762249	4.152062	0.000000
6	Ge	2.425364	2.865756	4.152062	4.049997	2.750159
7	Ge	4.177690	4.049633	2.751123	2.865756	4.151246
8	Ge	5.501990	4.177690	4.212218	2.425364	3.740979
9	Ge	2.954475	2.624663	2.511660	2.431097	5.119586
10	Ge	2.955136	4.267078	2.512185	4.150036	5.119035
11	Ge	4.724813	4.150632	5.119586	4.267065	2.511660
12	Ge	4.724082	2.430154	5.119035	2.625315	2.512185

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.861546	0.000000			
8	Ge	4.177894	2.425412	0.000000		
9	Ge	4.267065	4.150632	4.724813	0.000000	
10	Ge	2.625315	2.430154	4.724082	3.949160	0.000000
11	Ge	2.431097	2.624663	2.954475	5.642134	4.029244
12	Ge	4.150036	4.267078	2.955136	4.029244	5.641602

		11	12
11	Ge	0.000000	
12	Ge	3.949160	0.000000



6-1.1 Cuboh – O_h ^{T} → C_i [HE]

- 24900.3234982 (+37.24 kcal/mol)

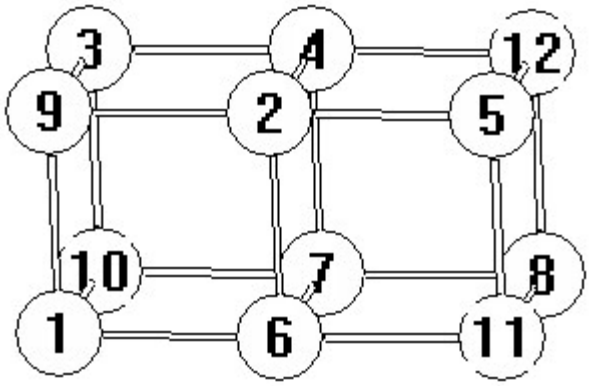
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.588058	0.000000			
3	Ge	3.616110	3.587817	0.000000		
4	Ge	4.416325	2.594872	2.498552	0.000000	
5	Ge	5.613991	2.498552	5.612128	3.587817	0.000000
6	Ge	2.498552	2.591401	4.416325	3.667250	3.588058
7	Ge	3.587817	3.667250	3.588058	2.591401	4.416325
8	Ge	5.612128	4.416325	5.613991	3.588058	3.616110
9	Ge	2.558211	2.498643	2.556426	3.588975	4.996936
10	Ge	2.556426	4.416781	2.558211	3.587550	6.168398
11	Ge	4.996936	3.587550	6.168398	4.416781	2.558211
12	Ge	6.168398	3.588975	4.996936	2.498643	2.556426

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.594872	0.000000			
8	Ge	3.587817	2.498552	0.000000		
9	Ge	3.587550	4.416781	6.168398	0.000000	
10	Ge	3.588975	2.498643	4.996936	3.617081	0.000000
11	Ge	2.498643	3.588975	2.556426	5.613442	5.613680
12	Ge	4.416781	3.587550	2.558211	5.613680	5.613442

		11	12
11	Ge	0.000000	
12	Ge	3.617081	0.000000



6-1.1 Cuboh – O_h → D_2 [20-2]

- 24898.6044534 (+7.98 kcal/mol)

Ge_{12} – 7-1_Anticuboct-D_{3h}

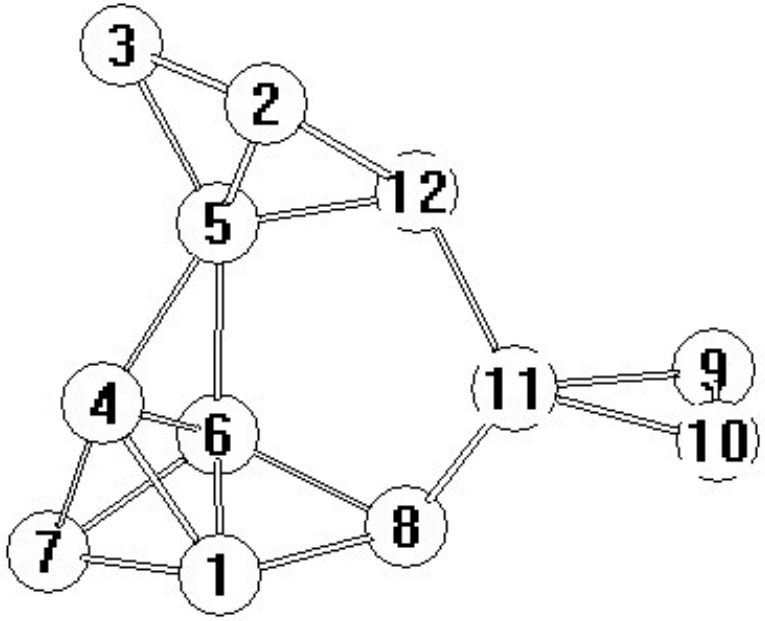
Charge 6-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	5.945072	0.000000			
3	Ge	6.454556	2.406075	0.000000		
4	Ge	2.518877	4.333719	4.284376	0.000000	
5	Ge	4.240003	2.796474	2.563662	2.700724	0.000000
6	Ge	2.618699	5.511579	5.309187	2.743341	2.913711
7	Ge	2.613117	6.869104	6.416199	2.725632	4.551619
8	Ge	2.652738	6.179462	6.890525	4.266648	4.346105
9	Ge	6.520505	6.924579	8.223062	7.495654	6.219526
10	Ge	6.237072	6.782701	8.581932	7.395495	6.677990
11	Ge	4.192471	4.846386	6.252236	4.959138	4.103415
12	Ge	5.147584	2.707260	3.956114	4.533414	2.478661

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.486653	0.000000			
8	Ge	2.612217	4.287292	0.000000		
9	Ge	6.036858	8.250083	4.137035	0.000000	
10	Ge	6.672217	8.496018	4.482681	2.360349	0.000000
11	Ge	4.149837	6.142623	2.523253	2.702133	2.656115
12	Ge	4.281393	6.377085	4.242084	4.338804	4.744175

		11	12
11	Ge	0.000000	
12	Ge	2.614382	0.000000



7-1.1 Anticuboct – D_{3h} → C_1 [30-1]

- 24899.0433125 (**+0.00 kcal/mol**)

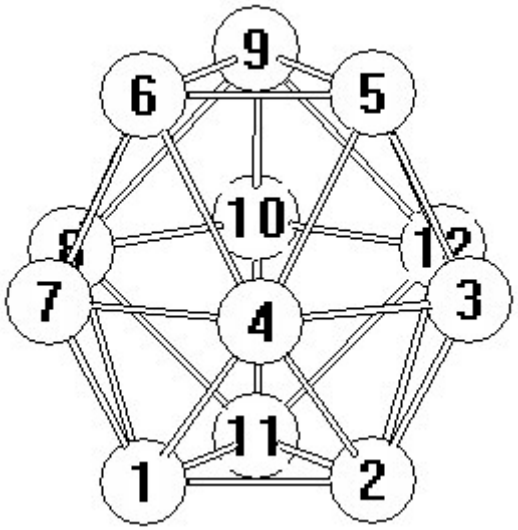
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.591650	0.000000			
3	Ge	4.351893	2.571922	0.000000		
4	Ge	3.085727	3.085727	2.597269	0.000000	
5	Ge	5.189765	4.496333	2.571922	3.085727	0.000000
6	Ge	4.496333	5.189765	4.351893	3.085727	2.591650
7	Ge	2.571922	4.351893	4.755347	2.597269	4.351893
8	Ge	3.085727	4.513938	5.163465	4.188037	4.513938
9	Ge	5.189765	5.189765	4.351893	4.513938	2.591650
10	Ge	4.351893	4.351893	4.755347	5.163465	4.351893
11	Ge	2.591650	2.591650	4.351893	4.513938	5.189765
12	Ge	4.513938	3.085727	2.597269	4.188037	3.085727

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.571922	0.000000			
8	Ge	3.085727	2.597269	0.000000		
9	Ge	2.591650	4.351893	3.085727	0.000000	
10	Ge	4.351893	4.755347	2.597269	2.571922	0.000000
11	Ge	5.189765	4.351893	3.085727	4.496333	2.571922
12	Ge	4.513938	5.163465	4.188037	3.085727	2.597269

		11	12
11	Ge	0.000000	
12	Ge	3.085727	0.000000



7-1 Anticuboct – D_{3h} [T] [HE]

- 24899.8821675 (+47.70 kcal/mol)

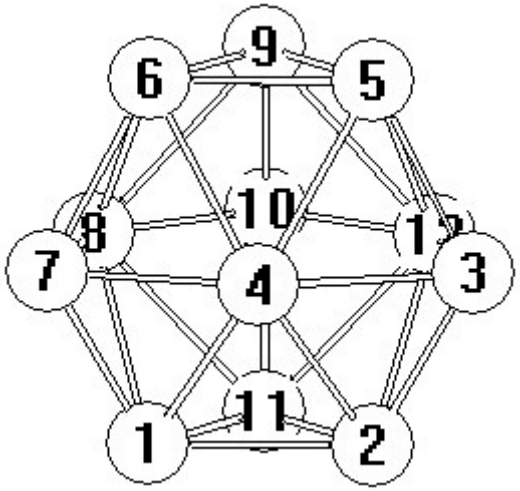
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.592592	0.000000			
3	Ge	4.383030	2.536035	0.000000		
4	Ge	2.942385	2.942385	2.611527	0.000000	
5	Ge	5.016730	4.294886	2.536035	2.942385	0.000000
6	Ge	4.294886	5.016730	4.383030	2.942385	2.592592
7	Ge	2.536035	4.383030	4.929230	2.611527	4.383030
8	Ge	2.942385	4.350312	5.132404	3.960354	4.350312
9	Ge	5.016730	5.016730	4.383030	4.350312	2.592592
10	Ge	4.383030	4.383030	4.929230	5.132404	4.383030
11	Ge	2.592592	2.592592	4.383030	4.350312	5.016730
12	Ge	4.350312	2.942385	2.611527	3.960354	2.942385

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.536035	0.000000			
8	Ge	2.942385	2.611527	0.000000		
9	Ge	2.592592	4.383030	2.942385	0.000000	
10	Ge	4.383030	4.929230	2.611527	2.536035	0.000000
11	Ge	5.016730	4.383030	2.942385	4.294886	2.536035
12	Ge	4.350312	5.132404	3.960354	2.942385	2.611527

		11	12
11	Ge	0.000000	
12	Ge	2.942385	0.000000



7-1 Anticuboct – D_{3h} [HE]

- 24900.3723225 (+48.61 kcal/mol)

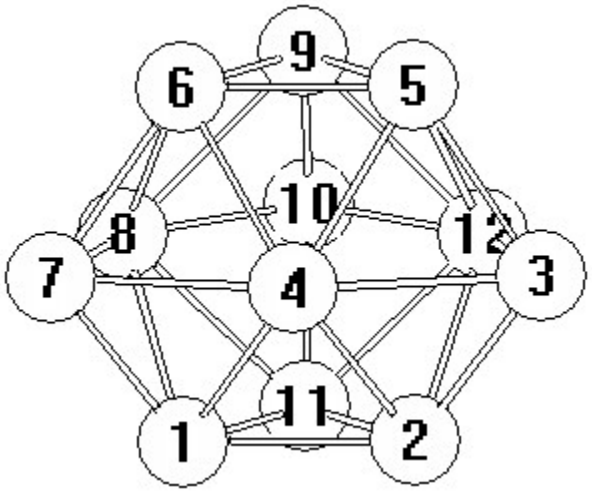
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.520585	0.000000			
3	Ge	4.452351	2.534185	0.000000		
4	Ge	2.789852	2.789852	2.758175	0.000000	
5	Ge	4.649405	3.906868	2.534185	2.789852	0.000000
6	Ge	3.906868	4.649405	4.452351	2.789852	2.520585
7	Ge	2.534185	4.452351	5.316755	2.758175	4.452351
8	Ge	2.789852	4.206398	5.339672	3.931828	4.206398
9	Ge	4.649405	4.649405	4.452351	4.206398	2.520585
10	Ge	4.452351	4.452351	5.316755	5.339672	4.452351
11	Ge	2.520585	2.520585	4.452351	4.206398	4.649405
12	Ge	4.206398	2.789852	2.758175	3.931828	2.789852

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.534185	0.000000			
8	Ge	2.789852	2.758175	0.000000		
9	Ge	2.520585	4.452351	2.789852	0.000000	
10	Ge	4.452351	5.316755	2.758175	2.534185	0.000000
11	Ge	4.649405	4.452351	2.789852	3.906868	2.534185
12	Ge	4.206398	5.339672	3.931828	2.789852	2.758175

		11	12
11	Ge	0.000000	
12	Ge	2.789852	0.000000



7-1 Anticuboct – D_{3h} [T] [HE]

- 24900.3001192 (+51.91 kcal/mol)

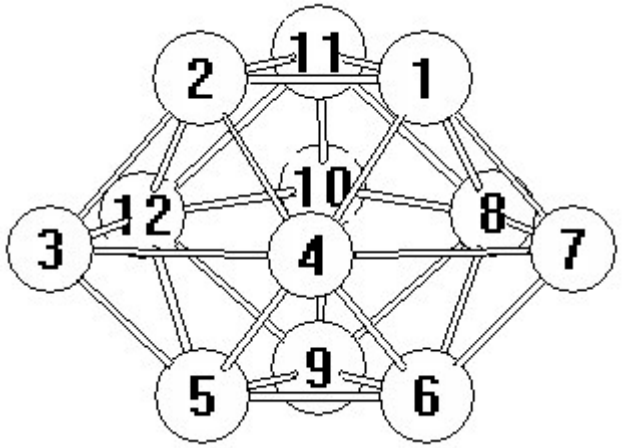
Charge 2+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.491311	0.000000			
3	Ge	4.610613	2.607318	0.000000		
4	Ge	2.645768	2.645768	2.956130	0.000000	
5	Ge	4.332075	3.544044	2.607318	2.645768	0.000000
6	Ge	3.544044	4.332075	4.610613	2.645768	2.491311
7	Ge	2.607318	4.610613	5.804033	2.956130	4.610613
8	Ge	2.645768	4.081597	5.589471	3.877215	4.081597
9	Ge	4.332075	4.332075	4.610613	4.081597	2.491311
10	Ge	4.610613	4.610613	5.804033	5.589471	4.610613
11	Ge	2.491311	2.491311	4.610613	4.081597	4.332075
12	Ge	4.081597	2.645768	2.956130	3.877215	2.645768

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.607318	0.000000			
8	Ge	2.645768	2.956130	0.000000		
9	Ge	2.491311	4.610613	2.645768	0.000000	
10	Ge	4.610613	5.804033	2.956130	2.607318	0.000000
11	Ge	4.332075	4.610613	2.645768	3.544044	2.607318
12	Ge	4.081597	5.589471	3.877215	2.645768	2.956130

		11	12
11	Ge	0.000000	
12	Ge	2.645768	0.000000



7-1 Anticuboct – D_{3h} [HE]

- 24899.7116791 (+42.13 kcal/mol)

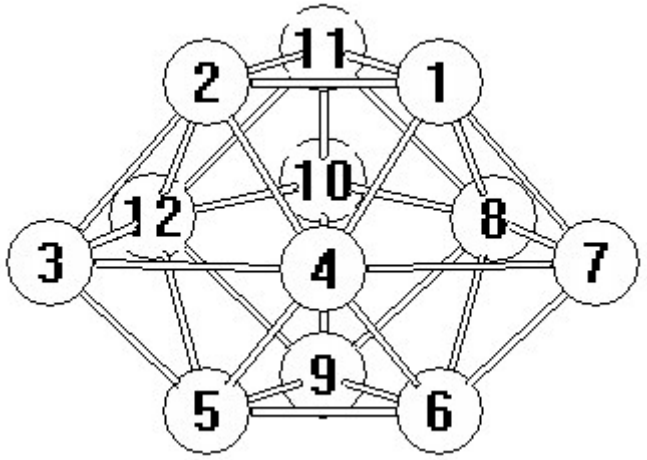
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.574505	0.000000			
3	Ge	4.793253	2.724791	0.000000		
4	Ge	2.668535	2.668535	3.050469	0.000000	
5	Ge	4.506704	3.698960	2.724791	2.668535	0.000000
6	Ge	3.698960	4.506704	4.793253	2.668535	2.574505
7	Ge	2.724791	4.793253	6.040300	3.050469	4.793253
8	Ge	2.668535	4.099943	5.660070	3.763229	4.099943
9	Ge	4.506704	4.506704	4.793253	4.099943	2.574505
10	Ge	4.793253	4.793253	6.040300	5.660070	4.793253
11	Ge	2.574505	2.574505	4.793253	4.099943	4.506704
12	Ge	4.099943	2.668535	3.050469	3.763229	2.668535

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.724791	0.000000			
8	Ge	2.668535	3.050469	0.000000		
9	Ge	2.574505	4.793253	2.668535	0.000000	
10	Ge	4.793253	6.040300	3.050469	2.724791	0.000000
11	Ge	4.506704	4.793253	2.668535	3.698960	2.724791
12	Ge	4.099943	5.660070	3.763229	2.668535	3.050469

		11	12
11	Ge	0.000000	
12	Ge	2.668535	0.000000



7-1 Anticuboct – D_{3h} [T] [HE]

- 24898.5565942 (+38.01 kcal/mol)

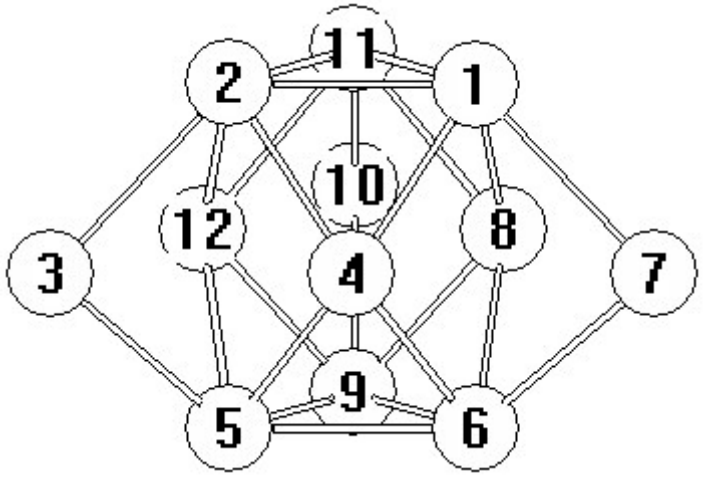
Charge 6+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.781953	0.000000			
3	Ge	5.339753	3.071985	0.000000		
4	Ge	2.687078	2.687078	3.428504	0.000000	
5	Ge	4.831790	3.950561	3.071985	2.687078	0.000000
6	Ge	3.950561	4.831790	5.339753	2.687078	2.781953
7	Ge	3.071985	5.339753	6.857008	3.428504	5.339753
8	Ge	2.687078	4.093693	5.938343	3.428503	4.093693
9	Ge	4.831790	4.831790	5.339753	4.093693	2.781953
10	Ge	5.339753	5.339753	6.857008	5.938343	5.339753
11	Ge	2.781953	2.781953	5.339753	4.093693	4.831790
12	Ge	4.093693	2.687078	3.428504	3.428503	2.687078

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	3.071985	0.000000			
8	Ge	2.687078	3.428504	0.000000		
9	Ge	2.781953	5.339753	2.687078	0.000000	
10	Ge	5.339753	6.857008	3.428504	3.071985	0.000000
11	Ge	4.831790	5.339753	2.687078	3.950561	3.071985
12	Ge	4.093693	5.938343	3.428503	2.687078	3.428504

		11	12
11	Ge	0.000000	
12	Ge	2.687078	0.000000



7-1 Anticuboct – D_{3h} [HE]

- 24896.8890450 (+98.21 kcal/mol)

Ge_{12} – 7-2_Centaur-C_{2v}

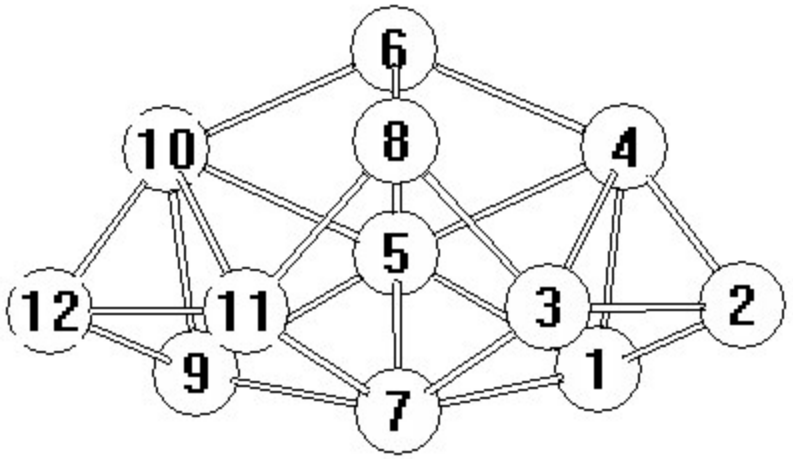
Charge 4-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.589294	0.000000			
3	Ge	3.243858	2.481248	0.000000		
4	Ge	2.586156	2.520471	3.154614	0.000000	
5	Ge	2.667791	4.650206	4.172907	3.092913	0.000000
6	Ge	4.239936	5.028404	4.312474	2.783097	2.504240
7	Ge	2.741963	4.028722	2.580838	3.970160	2.795681
8	Ge	4.303208	4.325428	2.548641	3.223611	3.526816
9	Ge	4.466338	6.404337	5.052323	5.420678	2.667791
10	Ge	5.420678	6.737164	5.198200	5.081467	3.092913
11	Ge	5.052323	5.653541	3.359206	5.198200	4.172907
12	Ge	6.404337	7.682154	5.653541	6.737164	4.650206

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.185836	0.000000			
8	Ge	2.479492	3.202101	0.000000		
9	Ge	4.239936	2.741963	4.303208	0.000000	
10	Ge	2.783097	3.970160	3.223611	2.586156	0.000000
11	Ge	4.312474	2.580838	2.548641	3.243858	3.154614
12	Ge	5.028404	4.028722	4.325428	2.589294	2.520471

		11	12
11	Ge	0.000000	
12	Ge	2.481248	0.000000



7-2.1 Centaur – C_{2v} → C_s [HE]

- 24899.9171025 (+25.77 kcal/mol)

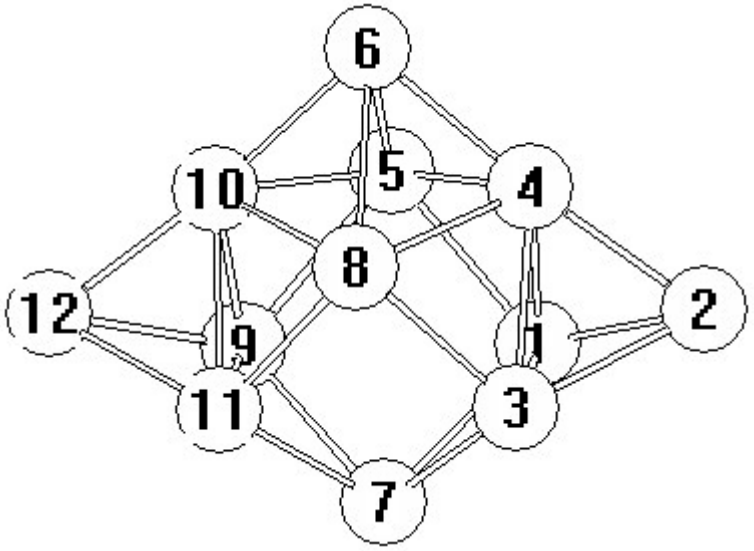
Charge 2-

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.574401	0.000000			
3	Ge	2.713809	2.574401	0.000000		
4	Ge	2.605459	2.417203	2.605459	0.000000	
5	Ge	2.598224	4.384629	4.210988	2.732309	0.000000
6	Ge	4.431951	4.850585	4.431951	2.439133	2.849899
7	Ge	2.620029	4.358322	2.620029	4.111655	3.900899
8	Ge	4.210988	4.384629	2.598224	2.732309	4.046582
9	Ge	3.374722	5.642127	4.330532	4.351974	2.598224
10	Ge	4.351974	5.721585	4.351974	3.600669	2.732309
11	Ge	4.330532	5.642127	3.374722	4.351974	4.210988
12	Ge	5.642127	7.469076	5.642127	5.721585	4.384629

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	5.342203	0.000000			
8	Ge	2.849899	3.900899	0.000000		
9	Ge	4.431951	2.620029	4.210988	0.000000	
10	Ge	2.439133	4.111655	2.732309	2.605459	0.000000
11	Ge	4.431951	2.620029	2.598224	2.713809	2.605459
12	Ge	4.850585	4.358322	4.384629	2.574401	2.417203

		11	12
11	Ge	0.000000	
12	Ge	2.574401	0.000000



7-2 Centaur – C_{2v} [26-1]

- 24900.4497809 (**+0.00 kcal/mol**)

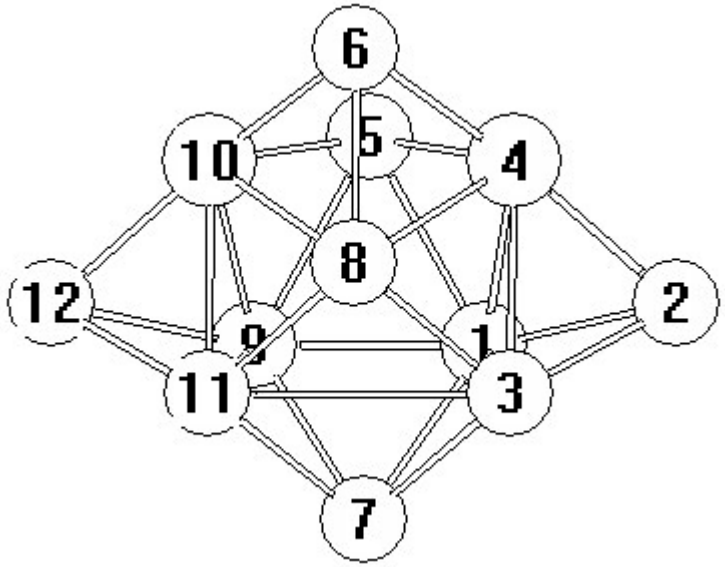
Charge
0

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.690066	0.000000			
3	Ge	2.884752	2.443008	0.000000		
4	Ge	2.816584	2.411332	2.739088	0.000000	
5	Ge	2.636584	4.219456	4.366913	2.592766	0.000000
6	Ge	4.818718	4.819072	4.207492	2.517012	3.474958
7	Ge	2.758533	4.220155	2.544851	4.341118	4.512143
8	Ge	4.184744	4.236836	2.457920	2.847236	4.175850
9	Ge	2.559769	5.000422	4.110695	4.073509	2.636584
10	Ge	4.073509	5.412778	4.340222	3.383246	2.592766
11	Ge	4.110695	5.405860	3.350310	4.340222	4.366913
12	Ge	5.000422	6.941158	5.405860	5.412778	4.219456

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	5.522259	0.000000			
8	Ge	2.462680	3.708295	0.000000		
9	Ge	4.818718	2.758533	4.184744	0.000000	
10	Ge	2.517012	4.341118	2.847236	2.816584	0.000000
11	Ge	4.207492	2.544851	2.457920	2.884752	2.739088
12	Ge	4.819072	4.220155	4.236836	2.690066	2.411332

		11	12
11	Ge	0.000000	
12	Ge	2.443008	0.000000



7-2.1 Centaur – C_{2v} → C_s [24-1]

- 24900.3828387 (**+0.00 kcal/mol**)

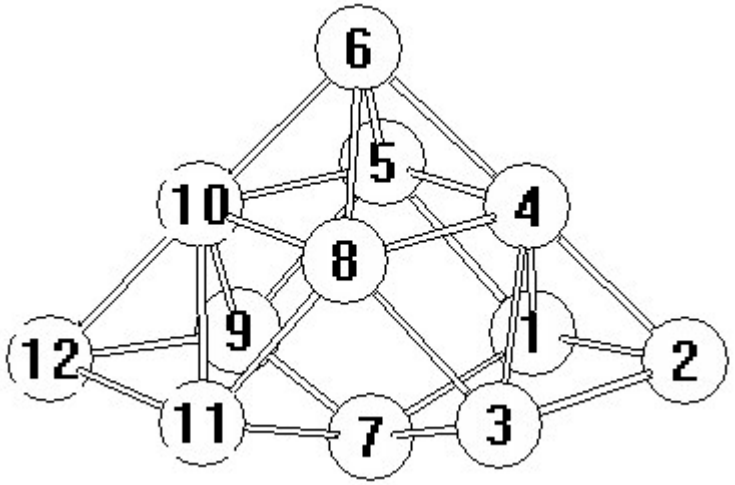
Charge 2+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.655667	0.000000			
3	Ge	3.687859	2.655667	0.000000		
4	Ge	2.716530	2.467628	2.716530	0.000000	
5	Ge	2.532533	4.393124	4.562363	2.676254	0.000000
6	Ge	4.534697	5.044738	4.534697	2.577372	2.710467
7	Ge	2.561691	3.653947	2.561691	3.229043	3.249002
8	Ge	4.562363	4.393124	2.532533	2.676254	3.905092
9	Ge	3.290624	5.511849	4.942521	4.406541	2.532533
10	Ge	4.406541	5.658940	4.406541	3.658295	2.676254
11	Ge	4.942521	5.511849	3.290624	4.406541	4.562363
12	Ge	5.511849	7.089207	5.511849	5.658940	4.393124

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	4.476785	0.000000			
8	Ge	2.710467	3.249002	0.000000		
9	Ge	4.534697	2.561691	4.562363	0.000000	
10	Ge	2.577372	3.229043	2.676254	2.716530	0.000000
11	Ge	4.534697	2.561691	2.532533	3.687859	2.716530
12	Ge	5.044738	3.653947	4.393124	2.655667	2.467628

		11	12
11	Ge	0.000000	
12	Ge	2.655667	0.000000



7-2 Centaur – C_{2v} [22-4]

- 24899.7652239 (+8.54 kcal/mol)

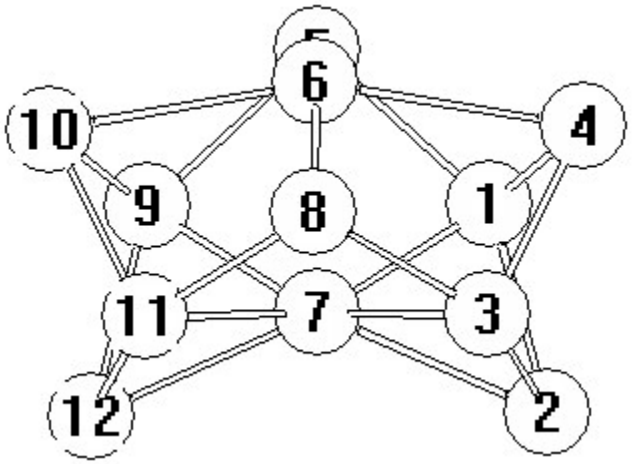
Charge 4+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	2.570225	0.000000			
3	Ge	3.409581	2.570225	0.000000		
4	Ge	2.555173	3.423968	2.555173	0.000000	
5	Ge	2.583254	4.905568	4.883421	3.892172	0.000000
6	Ge	3.321002	4.682889	3.321002	3.015654	2.583814
7	Ge	2.631136	2.806782	2.631136	3.693039	3.318068
8	Ge	4.883421	4.905568	2.583254	3.892172	5.037157
9	Ge	3.812650	5.095107	5.114836	5.399510	2.583254
10	Ge	5.399510	6.469019	5.399510	5.934401	3.892172
11	Ge	5.114836	5.095107	3.812650	5.399510	4.883421
12	Ge	5.095107	5.076273	5.095107	6.469019	4.905568

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.737107	0.000000			
8	Ge	2.583814	3.318068	0.000000		
9	Ge	3.321002	2.631136	4.883421	0.000000	
10	Ge	3.015654	3.693039	3.892172	2.555173	0.000000
11	Ge	3.321002	2.631136	2.583254	3.409581	2.555173
12	Ge	4.682889	2.806782	4.905568	2.570225	3.423968

		11	12
11	Ge	0.000000	
12	Ge	2.570225	0.000000



7-2 Centaur – C_{2v} [20-1]

- 24898.6171659 (**+0.00 kcal/mol**)

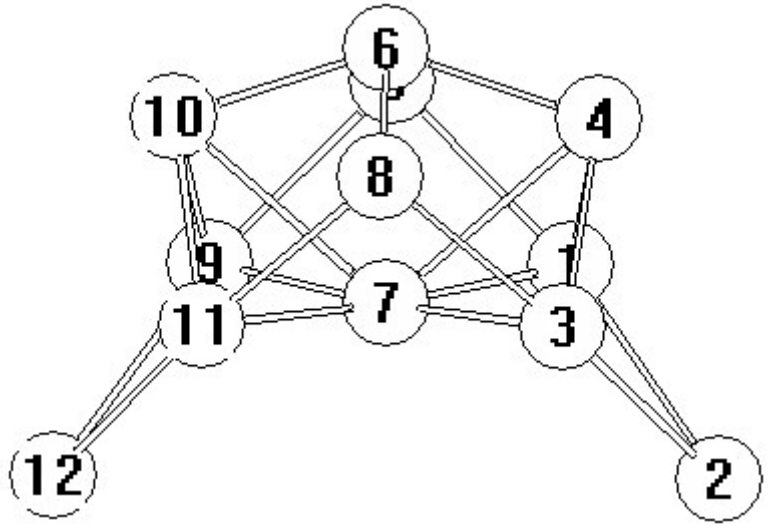
Charge 6+

Distance matrix (angstroms):

		1	2	3	4	5
1	Ge	0.000000				
2	Ge	3.128768	0.000000			
3	Ge	3.302378	3.128768	0.000000		
4	Ge	2.627483	4.286539	2.627483	0.000000	
5	Ge	2.893510	5.966408	5.011461	3.460629	0.000000
6	Ge	3.817131	6.096261	3.817131	2.479252	2.692474
7	Ge	2.599693	4.176813	2.599693	3.158482	3.217906
8	Ge	5.011461	5.966408	2.893510	3.460629	5.069783
9	Ge	4.011622	6.273189	5.196038	5.077295	2.893510
10	Ge	5.077295	7.283477	5.077295	4.705143	3.460629
11	Ge	5.196038	6.273189	4.011622	5.077295	5.011461
12	Ge	6.273189	7.369515	6.273189	7.283477	5.966408

		6	7	8	9	10
6	Ge	0.000000				
7	Ge	2.889834	0.000000			
8	Ge	2.692474	3.217906	0.000000		
9	Ge	3.817131	2.599693	5.011461	0.000000	
10	Ge	2.479252	3.158482	3.460629	2.627483	0.000000
11	Ge	3.817131	2.599693	2.893510	3.302378	2.627483
12	Ge	6.096261	4.176813	5.966408	3.128768	4.286539

		11	12
11	Ge	0.000000	
12	Ge	3.128768	0.000000



7-2 Centaur – C_{2v} [18-2]

- 24896.9534539 (+57.80 kcal/mol)

[HE] = high energy structure

Table S2. Energies of the bonding molecular orbitals of Ge_{12} and Ge_{12}^{2-}

Ge_{12}^{0}		Ge_{12}^{2-}	
No.	Energy	No.	Energy
169.	-0.67639	169.	-0.39347
170.	-0.61071	170.	-0.32114
171.	-0.59320	171.	-0.32113
172.	-0.59196	172.	-0.32100
173.	-0.48796	173.	-0.20599
174.	-0.48746	174.	-0.20598
175.	-0.47686	175.	-0.20589
176.	-0.47656	176.	-0.20587
177.	-0.46407	177.	-0.20579
178.	-0.38210	178.	-0.10335
179.	-0.38199	179.	-0.10331
180.	-0.35077	180.	-0.10313
181.	-0.30860	181.	-0.03685
182.	-0.30014	182.	-0.02567
183.	-0.29945	183.	-0.02564
184.	-0.29070	184.	-0.02557
185.	-0.29069	185.	-0.02556
186.	-0.23282	186.	0.03127
187.	-0.23242	187.	0.03127
188.	-0.22797	188.	0.03142
189.	-0.22769	189.	0.05267
190.	-0.21888	190.	0.05268
191.	-0.21553	191.	0.05271
192.	-0.21538	192.	0.05271
193.	-0.14253 **	193.	0.05289

** Empty antibonding orbital.