

Density Functional Theory Study of Eight-Atom Germanium Clusters: Effect of Electron Count on Cluster Geometry

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Supporting Information

Table S1. Energies of the optimized Ge₁₁^z structures ($z = 0, \pm 2, \pm 4, \pm 6$)

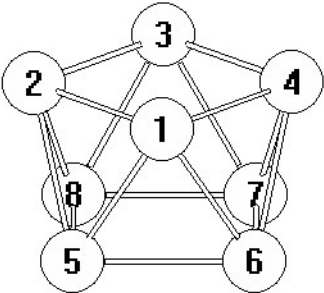
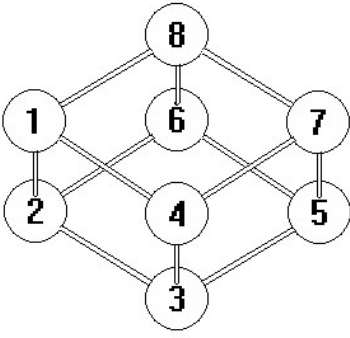
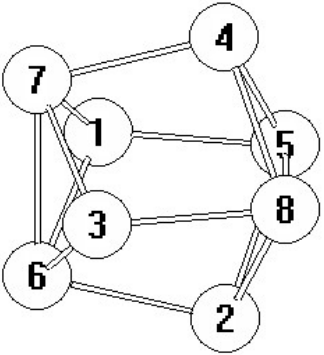
Table S2. Details of the optimized Ge₁₁^z structures ($z = 0, \pm 2, \pm 4, \pm 6$) structures including all interatomic distances (Å)

Table S1. Energies of the optimized Ge₁₁^z structures (z = 0, ±2, ±4, ±6)

	-6	-4	-2	0	+2	+4	+6
1.O_h	-16614.7266711 +0.92 D_{2h} 22-2	-16615.7444045 +15.65 C_i 20-4	-16616.2918019 0.0 T_d 18-1	-16616.177172 ^T +40.55	-16615.615592 +0.01 C₁ 14-1	-16614.2396877 +101.93 i53t_{2g}	-16612.3838998 +193.10
2.D_{4d}	-16614.7281345 0.0 22-1	-16615.745428 ^T i26 e ₂ +15.0 D_{4d} 20-3T	-16616.2756121 i61.5a ₂ +10.1 C_{2v} 18-3	-16616.238183 +2.77 16-1	-16615.5912224 +15.30 C₂ 14-5	-16614.3882392 +8.72 C₁ 12-2	-16612.691628^T 0.0 10-1T
3.1.D_{3h}	splits	splits	-16616.2241202 +42.5 i58a₁”, i53e’	-16616.2055803 +22.73 C_s i11.6	-16615.5912488 +15.28 C₂ 14-5	-16614.3686935 +20.99 C_s 12-5	splits into 1+3+3+1
4.3.D_{3d}	-16614.692216 ^T +22.54 22-4T	-16615.7444233 +15.64 20-4	-16616.2679824 +14.95 18-6	-16616.2248873 ^T +10.61 16-6	-16615.5975928 +11.30 14-3	-16614.2887581 +71.2 i53e_g, i50a_{2u}	splits into 1+[3+3]+1
5. D_{2d}	-16614.712959 ^T +9.52	-16615.7649156 +2.78 20-2	-16616.2856615 +3.85 18-2	-16616.225286 +10.36 16-5	-16615.5912214 +15.30 C₂ 14-5	-16614.3692861 +20.61 S₄ 12-4	splits into 2+4+2
6. D_{6h}	splits	splits	-16616.2297515 +38.93	-16616.189109 ^T +33.06 i63e_{2u}	-16615.6080893 +4.71 C_{2v} 14-2	-16614.3594325 +26.80 C_{2v}	splits
7. T_d	-16614.7130282 ^T +9.48 D_{2d} 22-3T	-16615.7648872 +2.80 D_{2d} 20-2	-16616.2917107 +0.05 18-1	-16616.2333611 +5.29 C₂ 16-3	-16615.6081699 +4.66 C₁ 14-2	-16614.3692218 +20.66 C₂	splits
8.nido_C_{2v}	-16614.8542466 (i1816.50)splits	-16615.7693482 0.0 20-1	-16616.2856275 +3.87 18-2	-16616.2417977 0.0 C_s 16-1	-16615.6155922 0.01 C₁ 14-1	-16614.3680232 +21.41	splits
9.cpb_C_s	nc	-16615.7648883 +2.79 C_s 20-2	-16616.2697783 +13.82 18-5	-16616.2332843 +5.34 16-4	-16615.6156026 0.0	-16614.3594207 +26.80 C_s	nc
10.dctp_C_s	nc	-16615.7649304 +2.77 20-2	-16616.271993 i39a” +12.43 18-4	-16616.2417968 0.0 C₁ 16-1	-16615.5849687 i74a”, i49a” +19.22	-16614.3881185 +8.80 12-3	nc
11.dco_C_{2v}	-16614.7266709 +0.92 22-2	-16615.7649164 +2.78 C_s 20-2	-16616.2635202 +17.74 C_s 18-7	-16616.2333634 +5.29 16-3	-16615.5952594 i58.5a” +12.76 C_s 14-4	-16614.4021392 0.0 C_s 12-1	nc
12.dctp_C₂_v	splits	-16615.7649304 +2.77 C₂ 20-2	-16616.2856280 +3.87 C₂ 18-2	-16616.2417977 0.0 C₁ 16-1	-16615.5912215 +15.30 C₂ 14-5	-16614.3691904 +20.68 C₂	nc

nc= not calculated ; cpb=capped pentagonal bipyramid; dctp=dicapped trigonal prism; dco=dicapped octahedron

Table S2. Details of the optimized Ge_{11}^z structures ($z = 0, \pm 2, \pm 4, \pm 6$) structures including all interatomic distances (Å)

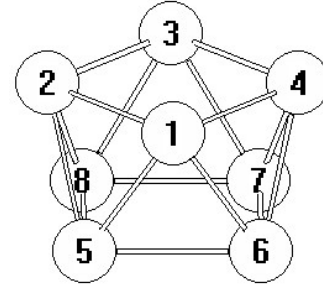
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22-2 E=-16614.7266711 12345 1 Ge 0.000000 2 Ge 2.748675 0.000000 3 Ge 3.846526 2.778451 0.000000 4 Ge 2.778451 3.846526 2.574322 0.000000 5 Ge 5.238708 4.459691 2.778451 3.846526 0.000000 6 Ge 3.846526 2.778451 3.310576 4.193691 2.778451 7 Ge 4.459691 5.238708 3.846526 2.778451 2.748675 8 Ge 2.778451 3.846526 4.193691 3.310576 3.846526 678 6 Ge 0.000000 7 Ge 3.846526 0.000000 8 Ge 2.574322 2.778451 0.000000						
22-3 E=-16614.713028 12345 1 Ge 0.000000 2 Ge 3.552265 0.000000 3 Ge 4.306372 3.552265 0.000000 4 Ge 3.552265 4.306372 3.552265 0.000000 5 Ge 2.774106 2.760444 4.535461 2.760444 0.000000 6 Ge 2.760444 2.774106 2.760444 4.535461 4.140776 7 Ge 2.760444 4.535461 2.760444 2.774106 4.140776 8 Ge 4.535461 2.760444 2.774106 2.760444 2.989697 678 6 Ge 0.000000 7 Ge 2.989697 0.000000 8 Ge 4.140776 4.140776 0.000000						

22-4T E=-16614.6922156																																																																																			
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20-3T

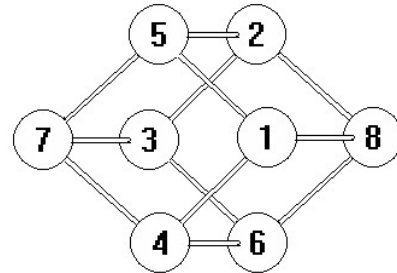
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3 Ge	3.896250	2.755065	0.000000		
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5 Ge	2.700701	2.700701	4.245964	4.245964	0.000000
6 Ge	2.700701	4.245964	4.245964	2.700701	2.755065
7 Ge	4.245964	4.245964	2.700701	2.700701	3.896250
8 Ge	4.245964	2.700701	2.700701	4.245964	2.755065
	6	7	8		
6 Ge	0.000000				
7 Ge	2.755065	0.000000			
8 Ge	3.896250	2.755065	0.000000		

**20-4**

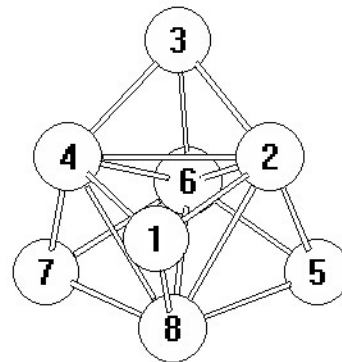
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2 Ge	3.364108	0.000000			
3 Ge	4.245116	2.589168	0.000000		
4 Ge	2.589168	4.245116	3.364108	0.000000	
5 Ge	2.589168	2.589168	3.364108	3.364108	0.000000
6 Ge	3.364108	3.364108	2.589168	2.589168	4.245116
7 Ge	4.035147	4.035147	2.665028	2.665028	2.665028
8 Ge	2.665028	2.665028	4.035147	4.035147	4.035147
	6	7	8		
6 Ge	0.000000				
7 Ge	4.035147	0.000000			
8 Ge	2.665028	5.361769	0.000000		

**18-1**

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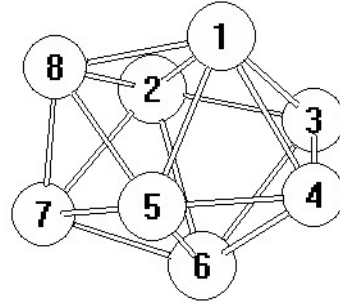
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5 Ge	4.100091	2.582168	4.100091	4.379218	0.000000
6 Ge	4.379218	3.051141	2.582168	3.051141	2.582168
7 Ge	4.100091	4.379218	4.100091	2.582168	4.100091
8 Ge	2.582168	3.051141	4.379218	3.051141	2.582168
	6	7	8		
6 Ge	0.000000				
7 Ge	2.582168	0.000000			
8 Ge	3.051141	2.582168	0.000000		



18-2

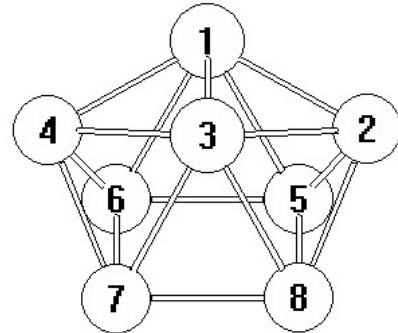
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2 Ge	2.927844	0.000000			
3 Ge	2.810673	2.588023	0.000000		
4 Ge	2.810673	4.069411	2.508630	0.000000	
5 Ge	2.927844	3.931325	4.069411	2.588023	0.000000
6 Ge	3.931325	2.927844	2.810673	2.810673	2.927844
7 Ge	4.069411	2.810673	4.428453	4.428453	2.810673
8 Ge	2.588023	2.810673	4.428453	4.428453	2.810673
	6	7	8		
6 Ge	0.000000				
7 Ge	2.588023	0.000000			
8 Ge	4.069411	2.508630	0.000000		

**18-3**

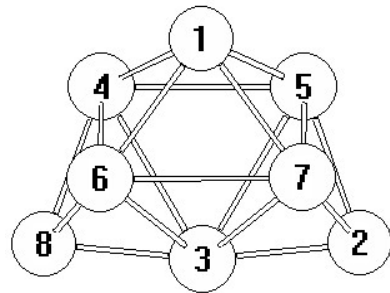
E=-16616.2756121

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2 Ge	2.719814	0.000000			
3 Ge	2.794135	2.719814	0.000000		
4 Ge	2.719814	4.481152	2.719814	0.000000	
5 Ge	2.845972	2.580708	4.041360	4.258043	0.000000
6 Ge	2.845972	4.258043	4.041360	2.580708	2.559805
7 Ge	4.041360	4.258043	2.845972	2.580708	3.903167
8 Ge	4.041360	2.580708	2.845972	4.258043	2.946542
	6	7	8		
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7 Ge	2.946542	0.000000			
8 Ge	3.903167	2.559805	0.000000		

**18-4**

E=-16616.2719923

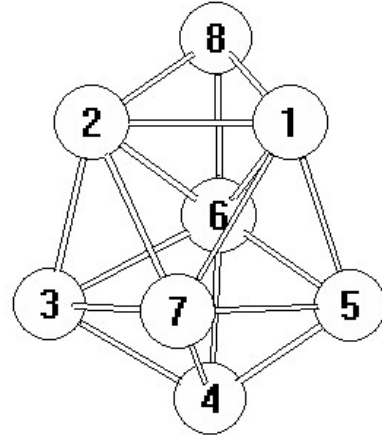
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1 Ge	0.000000				
2 Ge	4.362527	0.000000			
3 Ge	3.898252	2.447331	0.000000		
4 Ge	2.663936	4.663537	3.068147	0.000000	
5 Ge	2.664956	2.563134	3.067191	3.120032	0.000000
6 Ge	2.663936	4.663537	3.068147	2.781357	4.179931
7 Ge	2.664956	2.563134	3.067191	4.179931	2.781814
8 Ge	4.361656	4.863619	2.447718	2.563273	4.662697
	6	7	8		
6 Ge	0.000000				
7 Ge	3.120032	0.000000			
8 Ge	2.563273	4.662697	0.000000		



18-5

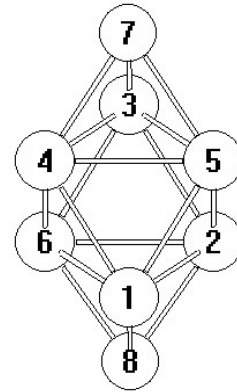
E=-16616.2697783

	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.769663	0.000000			
3 Ge	4.352017	2.707567	0.000000		
4 Ge	4.350491	4.350491	2.611740	0.000000	
5 Ge	2.707567	4.352017	4.191533	2.611740	0.000000
6 Ge	2.889273	2.889273	2.847941	2.609440	2.847941
7 Ge	3.072286	3.072286	2.638744	2.748086	2.638744
8 Ge	2.629138	2.629138	4.392046	4.977753	4.392046
	6	7	8		
6 Ge	0.000000				
7 Ge	3.350485	0.000000			
8 Ge	2.446451	4.680657	0.000000		

**18-6**

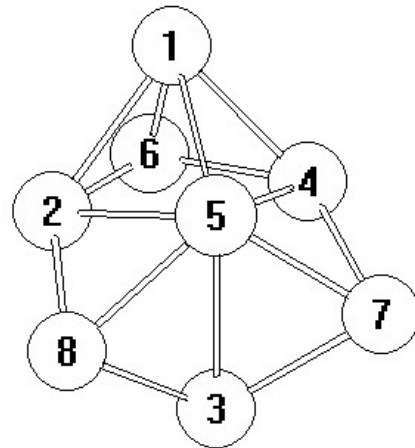
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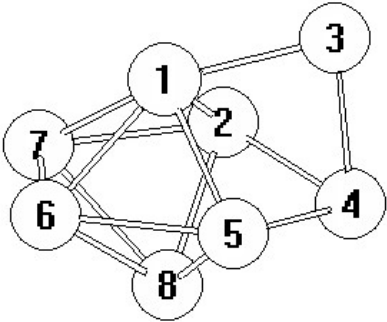
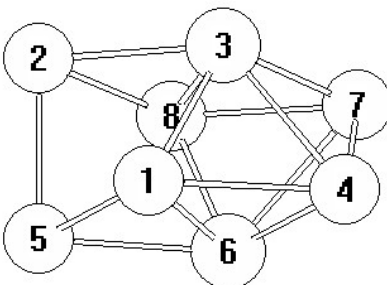
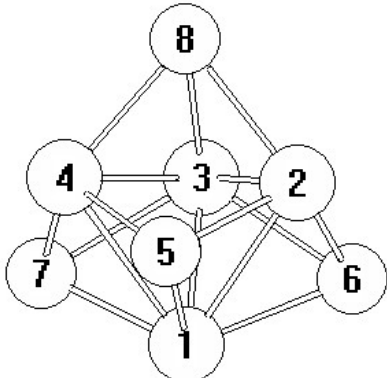
	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.913871	0.000000			
3 Ge	4.028019	2.781060	0.000000		
4 Ge	2.781060	4.028019	2.913871	0.000000	
5 Ge	2.781060	2.781060	2.913871	2.913871	0.000000
6 Ge	2.913871	2.913871	2.781060	2.781060	4.028019
7 Ge	4.429266	4.429266	2.524923	2.524923	2.524923
8 Ge	2.524923	2.524923	4.429266	4.429266	4.429266
	6	7	8		
6 Ge	0.000000				
7 Ge	4.429266	0.000000			
8 Ge	2.524923	5.980161	0.000000		

**18-7**

E=-16616.2635202

	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.618175	0.000000			
3 Ge	4.602755	3.278225	0.000000		
4 Ge	2.618175	3.280333	3.278225	0.000000	
5 Ge	2.767065	2.959662	2.887280	2.959662	0.000000
6 Ge	2.856306	2.487689	4.211189	2.487689	4.313990
7 Ge	4.357883	4.517078	2.488163	2.678930	2.542076
8 Ge	4.357883	2.678930	2.488163	4.517078	2.542076
	6	7	8		
6 Ge	0.000000				
7 Ge	4.865527	0.000000			
8 Ge	4.865527	4.032312	0.000000		

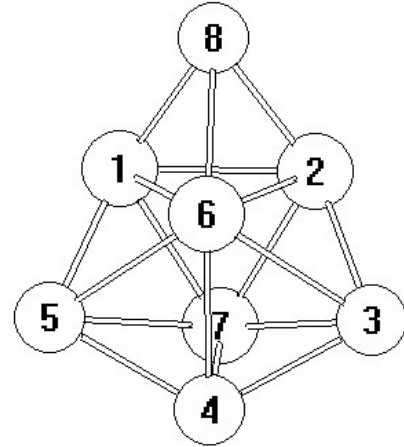


16-1 E=-16616.2417977																																																																																				
<table><tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1 Ge</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Ge</td><td>2.730058</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Ge</td><td>2.464019</td><td>3.319958</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Ge</td><td>3.227235</td><td>2.744726</td><td>2.508789</td><td>0.000000</td><td></td></tr><tr><td>5 Ge</td><td>2.731316</td><td>4.209885</td><td>3.319381</td><td>2.741597</td><td>0.000000</td></tr><tr><td>6 Ge</td><td>2.614507</td><td>4.297084</td><td>4.779652</td><td>4.530446</td><td>2.724513</td></tr><tr><td>7 Ge</td><td>2.614370</td><td>2.724426</td><td>4.780389</td><td>4.532413</td><td>4.298436</td></tr><tr><td>8 Ge</td><td>3.094891</td><td>2.777771</td><td>4.369918</td><td>2.819308</td><td>2.778137</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Ge</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Ge</td><td>2.624301</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Ge</td><td>2.725734</td><td>2.726691</td><td>0.000000</td><td></td><td></td></tr></table>								1	2	3	4	5	1 Ge	0.000000					2 Ge	2.730058	0.000000				3 Ge	2.464019	3.319958	0.000000			4 Ge	3.227235	2.744726	2.508789	0.000000		5 Ge	2.731316	4.209885	3.319381	2.741597	0.000000	6 Ge	2.614507	4.297084	4.779652	4.530446	2.724513	7 Ge	2.614370	2.724426	4.780389	4.532413	4.298436	8 Ge	3.094891	2.777771	4.369918	2.819308	2.778137		6	7	8			6 Ge	0.000000					7 Ge	2.624301	0.000000				8 Ge	2.725734	2.726691	0.000000		
	1	2	3	4	5																																																																															
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16-2 E=-16616.2381831																																																																																				
<table><tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1 Ge</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Ge</td><td>3.211497</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Ge</td><td>2.691805</td><td>2.660440</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Ge</td><td>2.786764</td><td>4.897491</td><td>2.792221</td><td>0.000000</td><td></td></tr><tr><td>5 Ge</td><td>2.709324</td><td>2.508086</td><td>3.755906</td><td>4.542522</td><td>0.000000</td></tr><tr><td>6 Ge</td><td>2.757220</td><td>3.760677</td><td>2.951606</td><td>2.488339</td><td>2.662841</td></tr><tr><td>7 Ge</td><td>4.332126</td><td>4.542621</td><td>2.487966</td><td>2.697452</td><td>4.896766</td></tr><tr><td>8 Ge</td><td>4.189975</td><td>2.712022</td><td>2.756045</td><td>4.331218</td><td>3.209980</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Ge</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Ge</td><td>2.792855</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Ge</td><td>2.691755</td><td>2.785867</td><td>0.000000</td><td></td><td></td></tr></table>								1	2	3	4	5	1 Ge	0.000000					2 Ge	3.211497	0.000000				3 Ge	2.691805	2.660440	0.000000			4 Ge	2.786764	4.897491	2.792221	0.000000		5 Ge	2.709324	2.508086	3.755906	4.542522	0.000000	6 Ge	2.757220	3.760677	2.951606	2.488339	2.662841	7 Ge	4.332126	4.542621	2.487966	2.697452	4.896766	8 Ge	4.189975	2.712022	2.756045	4.331218	3.209980		6	7	8			6 Ge	0.000000					7 Ge	2.792855	0.000000				8 Ge	2.691755	2.785867	0.000000		
	1	2	3	4	5																																																																															
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2 Ge	3.211497	0.000000																																																																																		
3 Ge	2.691805	2.660440	0.000000																																																																																	
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8 Ge	2.691755	2.785867	0.000000																																																																																	
16-3 E=-16616.2333611																																																																																				
<table><tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1 Ge</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Ge</td><td>2.970737</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Ge</td><td>2.742720</td><td>2.975880</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Ge</td><td>2.975880</td><td>3.224369</td><td>2.970737</td><td>0.000000</td><td></td></tr><tr><td>5 Ge</td><td>3.000393</td><td>2.526124</td><td>4.300740</td><td>2.528676</td><td>0.000000</td></tr><tr><td>6 Ge</td><td>2.582400</td><td>2.533579</td><td>2.583245</td><td>4.506798</td><td>4.356258</td></tr><tr><td>7 Ge</td><td>2.583245</td><td>4.506798</td><td>2.582400</td><td>2.533579</td><td>4.352947</td></tr><tr><td>8 Ge</td><td>4.300740</td><td>2.528676</td><td>3.000393</td><td>2.526124</td><td>3.461539</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Ge</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Ge</td><td>4.308524</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Ge</td><td>4.352947</td><td>4.356258</td><td>0.000000</td><td></td><td></td></tr></table>								1	2	3	4	5	1 Ge	0.000000					2 Ge	2.970737	0.000000				3 Ge	2.742720	2.975880	0.000000			4 Ge	2.975880	3.224369	2.970737	0.000000		5 Ge	3.000393	2.526124	4.300740	2.528676	0.000000	6 Ge	2.582400	2.533579	2.583245	4.506798	4.356258	7 Ge	2.583245	4.506798	2.582400	2.533579	4.352947	8 Ge	4.300740	2.528676	3.000393	2.526124	3.461539		6	7	8			6 Ge	0.000000					7 Ge	4.308524	0.000000				8 Ge	4.352947	4.356258	0.000000		
	1	2	3	4	5																																																																															
1 Ge	0.000000																																																																																			
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7 Ge	4.308524	0.000000																																																																																		
8 Ge	4.352947	4.356258	0.000000																																																																																	

16-4

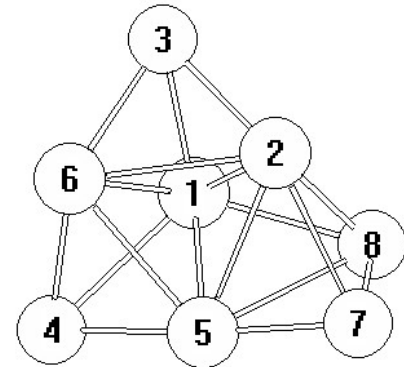
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	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.691598	0.000000			
3 Ge	4.255176	2.487333	0.000000		
4 Ge	3.818280	3.818280	2.554671	0.000000	
5 Ge	2.487333	4.255176	4.428484	2.554671	0.000000
6 Ge	2.862408	2.862408	2.959706	2.882727	2.959706
7 Ge	2.734047	2.734047	3.085702	2.683047	3.085702
8 Ge	2.494578	2.494578	4.440542	5.101839	4.440542
	6	7	8		
6 Ge	0.000000				
7 Ge	3.807572	0.000000			
8 Ge	2.774014	4.475680	0.000000		

**16-5**

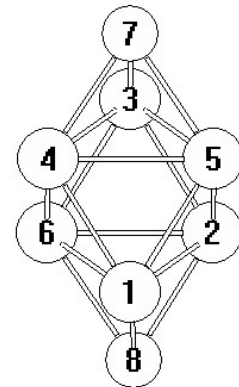
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	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.817997	0.000000			
3 Ge	2.720646	2.498605	0.000000		
4 Ge	3.000387	4.348676	4.488912	0.000000	
5 Ge	2.964471	2.787505	4.296040	2.470393	0.000000
6 Ge	2.793116	2.992378	2.489810	2.450064	2.909172
7 Ge	4.360114	2.804488	5.219853	4.885451	2.422179
8 Ge	2.802353	2.568097	4.298152	4.760409	3.052478
	6	7	8		
6 Ge	0.000000				
7 Ge	4.734040	0.000000			
8 Ge	4.646903	2.595922	0.000000		

**16-6T**

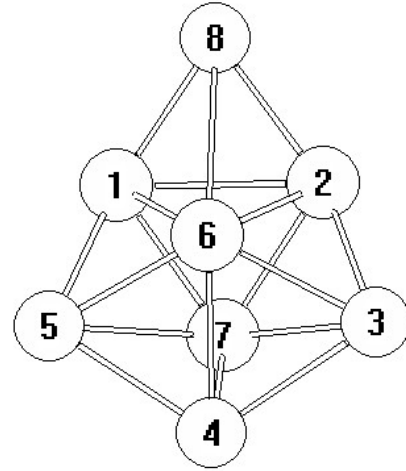
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	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.852379	0.000000			
3 Ge	3.929708	2.703060	0.000000		
4 Ge	2.703060	3.929708	2.852379	0.000000	
5 Ge	2.703060	2.703060	2.852379	2.852379	0.000000
6 Ge	2.852379	2.852379	2.703060	2.703060	3.929708
7 Ge	4.428963	4.428963	2.566080	2.566080	2.566080
8 Ge	2.566080	2.566080	4.428963	4.428963	4.428963
	6	7	8		
6 Ge	0.000000				
7 Ge	4.428963	0.000000			
8 Ge	2.566080	6.079339	0.000000		

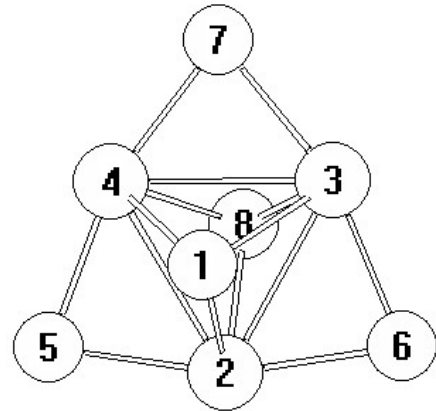


14-1**E=-16615.6156026**

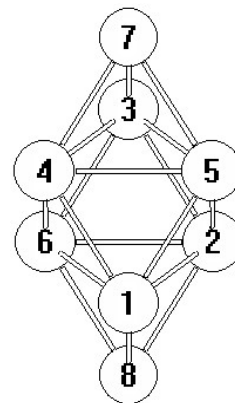
	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.902243	0.000000			
3 Ge	4.489876	2.612187	0.000000		
4 Ge	4.204450	4.204450	2.780862	0.000000	
5 Ge	2.612187	4.489876	4.594883	2.780862	0.000000
6 Ge	2.723023	2.723023	2.707054	2.808101	2.707054
7 Ge	2.607336	2.607336	2.958803	2.575417	2.958803
8 Ge	2.581009	2.581009	4.725453	5.696066	4.725453
	6	7	8		
6 Ge	0.000000				
7 Ge	2.920264	0.000000			
8 Ge	3.211128	4.294975	0.000000		

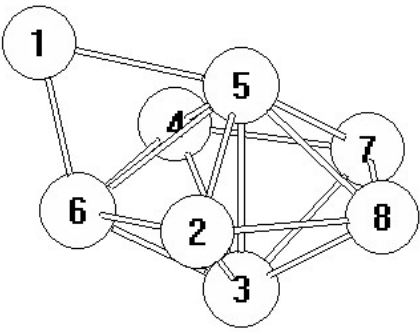
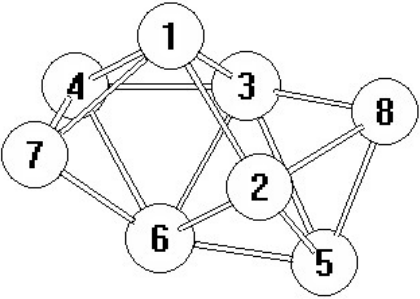
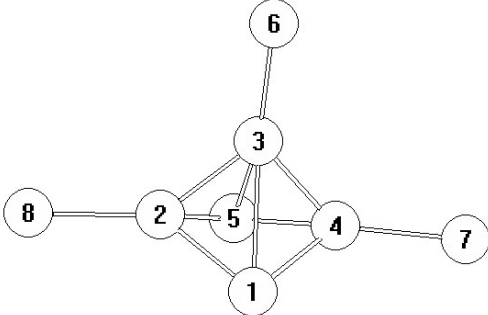
**14-2****E=-16615.6081699**

	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.750904	0.000000			
3 Ge	2.750158	3.105471	0.000000		
4 Ge	2.751145	3.103516	3.104674	0.000000	
5 Ge	3.537360	2.498851	4.648172	2.498855	0.000000
6 Ge	3.534373	2.499108	2.499277	4.646137	4.944388
7 Ge	3.535272	4.646970	2.499161	2.498954	4.944464
8 Ge	4.173092	2.750816	2.750307	2.750954	3.537452
	6	7	8		
6 Ge	0.000000				
7 Ge	4.944491	0.000000			
8 Ge	3.535130	3.536047	0.000000		

**14-3****E=-16615.5975928**

	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.850127	0.000000			
3 Ge	3.899434	2.661271	0.000000		
4 Ge	2.661271	3.899434	2.850127	0.000000	
5 Ge	2.661271	2.661271	2.850127	2.850127	0.000000
6 Ge	2.850127	2.850127	2.661271	2.661271	3.899434
7 Ge	4.516081	4.516081	2.678991	2.678991	2.678991
8 Ge	2.678991	2.678991	4.516081	4.516081	4.516081
	6	7	8		
6 Ge	0.000000				
7 Ge	4.516081	0.000000			
8 Ge	2.678991	6.319681	0.000000		



14-4 $E=-16615.5952594$						
	1	2	3	4	5	
1 Ge	0.000000					
2 Ge	3.615712	0.000000				
3 Ge	4.461365	2.877152	0.000000			
4 Ge	3.615712	4.590558	2.877152	0.000000		
5 Ge	2.795046	2.738701	2.876476	2.738701	0.000000	
6 Ge	2.450874	2.752178	2.470360	2.752178	2.789486	
7 Ge	5.191934	4.526284	2.734416	2.682740	2.722765	
8 Ge	5.191934	2.682740	2.734416	4.526284	2.722765	
	6	7	8			
6 Ge	0.000000					
7 Ge	4.264278	0.000000				
8 Ge	4.264278	2.895106	0.000000			
14-5 $E=-16615.5912488$						
	1	2	3	4	5	
1 Ge	0.000000					
2 Ge	2.687898	0.000000				
3 Ge	2.662472	3.326157	0.000000			
4 Ge	3.127718	4.582841	2.553625	0.000000		
5 Ge	4.582841	3.127718	2.891149	4.576517	0.000000	
6 Ge	3.326157	2.662472	2.742873	2.891149	2.553625	
7 Ge	2.675010	3.500572	3.860789	2.694992	4.940202	
8 Ge	3.500572	2.675010	2.520378	4.940202	2.694992	
	6	7	8			
6 Ge	0.000000					
7 Ge	2.520378	0.000000				
8 Ge	3.860789	5.269790	0.000000			
12-1 $E=-16614.4021392$						
	1	2	3	4	5	
1 Ge	0.000000					
2 Ge	2.615722	0.000000				
3 Ge	3.075471	2.522059	0.000000			
4 Ge	2.615722	3.599812	2.522059	0.000000		
5 Ge	3.464374	2.615390	3.076534	2.615390	0.000000	
6 Ge	5.441419	4.737593	2.615699	4.737593	5.440016	
7 Ge	4.843563	6.278429	4.863319	2.680499	4.843145	
8 Ge	4.843563	2.680499	4.863319	6.278429	4.843145	
	6	7	8			
6 Ge	0.000000					
7 Ge	6.358427	0.000000				
8 Ge	6.358427	8.954245	0.000000			

12-2 E=-16614.3882392							
	1	2	3	4	5		
1 Ge	0.000000						
2 Ge	2.762004	0.000000					
3 Ge	4.807640	2.462748	0.000000				
4 Ge	2.602763	3.211622	4.117614	0.000000			
5 Ge	2.636762	2.751021	5.189985	4.480176	0.000000		
6 Ge	2.602660	3.212658	4.118335	3.499553	4.480280		
7 Ge	3.775463	3.010128	2.459177	2.645591	5.392198		
8 Ge	7.629865	5.032254	2.886141	6.830770	7.499832		
	6	7	8				
6 Ge	0.000000						
7 Ge	2.645770	0.000000					
8 Ge	6.832095	5.090385	0.000000				
12-3 E=-16614.3881185							
	1	2	3	4	5		
1 Ge	0.000000						
2 Ge	4.091338	0.000000					
3 Ge	6.835926	2.747176	0.000000				
4 Ge	2.662543	2.590146	5.052155	0.000000			
5 Ge	4.565779	4.872798	6.721604	2.627946	0.000000		
6 Ge	2.662543	2.590146	5.052155	2.649933	5.061355		
7 Ge	4.565779	4.872798	6.721604	5.061355	7.061016		
8 Ge	2.714195	2.580892	4.943578	2.970044	5.375355		
	6	7	8				
6 Ge	0.000000						
7 Ge	2.627946	0.000000					
8 Ge	2.970044	5.375355	0.000000				
12-4 E=-16614.3692861							
	1	2	3	4	5		
1 Ge	0.000000						
2 Ge	2.654014	0.000000					
3 Ge	4.026494	3.033548	0.000000				
4 Ge	2.617844	4.894835	5.974446	0.000000			
5 Ge	2.654014	2.924929	4.894835	3.033548	0.000000		
6 Ge	2.924929	2.654014	2.617844	4.026494	2.654014		
7 Ge	4.894835	4.026494	5.201844	5.201844	2.617844		
8 Ge	3.033548	2.617844	5.201844	5.201844	4.026494		
	6	7	8				
6 Ge	0.000000						
7 Ge	3.033548	0.000000					
8 Ge	4.894835	5.974446	0.000000				

12-5 $E=-16614.3686935$					
	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.737290	0.000000			
3 Ge	5.290535	2.827522	0.000000		
4 Ge	4.850016	2.763006	2.455924	0.000000	
5 Ge	5.290535	2.827522	3.201423	3.832144	0.000000
6 Ge	4.850016	2.763006	3.832144	2.703099	2.455924
7 Ge	6.447245	4.723407	4.941082	2.777673	4.941082
8 Ge	4.779146	2.838666	2.762841	4.574826	2.762841
	6	7	8		
6 Ge	0.000000				
7 Ge	2.777673	0.000000			
8 Ge	4.574826	6.762918	0.000000		
12-6 $E=-16614.33594325$					
	1	2	3	4	5
1 Ge	0.000000				
2 Ge	2.726368	0.000000			
3 Ge	5.371244	2.726654	0.000000		
4 Ge	5.119946	3.498960	2.726735	0.000000	
5 Ge	5.371244	5.122680	5.372327	2.726735	0.000000
6 Ge	2.726368	3.500756	5.122680	3.498960	2.726654
7 Ge	3.534658	2.639373	3.536088	2.638529	3.536088
8 Ge	3.534658	2.639373	3.536088	2.638529	3.536088
	6	7	8		
6 Ge	0.000000				
7 Ge	2.639373	0.000000			
8 Ge	2.639373	3.395586	0.000000		
10-T $E=-16612.6916283$					
	1	2	3	4	5
1 Ge	0.000000				
2 Ge	5.749639	0.000000			
3 Ge	8.131217	5.749639	0.000000		
4 Ge	5.749639	8.131217	5.749639	0.000000	
5 Ge	3.162731	3.162731	7.533554	7.533554	0.000000
6 Ge	3.162731	7.533554	7.533554	3.162731	5.749639
7 Ge	7.533554	7.533554	3.162731	3.162731	8.131217
8 Ge	7.533554	3.162731	3.162731	7.533554	5.749639
	6	7	8		
6 Ge	0.000000				
7 Ge	5.749639	0.000000			
8 Ge	8.131217	5.749639	0.000000		