Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

$CSi_nGe_{4-n}^{2+}$ (n = 1-3): Prospective Systems Containing Planar Tetracoordinate Carbon (ptC)

Prasenjit Das,[a] Maya Khatun, [a] Anakuthil Anoop, [a,*] Pratim Kumar Chattaraj[a,*]

[a] *Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur 721302, India*

*E-mail: anoop@chem.iitkgp.ac.in (AA); pkc@chem.iitkgp.ac.in (PKC)

Supporting Information

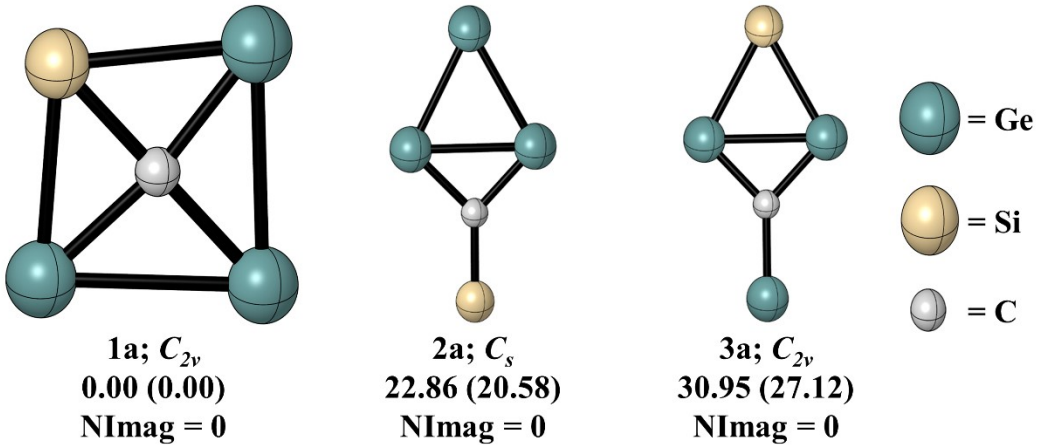

Figure S1. Low-lying isomers of $CSiGe_3^{2+}$ system on the PES using PyAR program. The values without and within parentheses are the relative energies in kcal/mol at PBE0-D3(BJ)/def2-TZVP and CCSD(T)/aug-cc-pVTZ methods, respectively. The number of imaginary frequencies (NImag) obtained for each stationary point is indicated underneath the geometries.

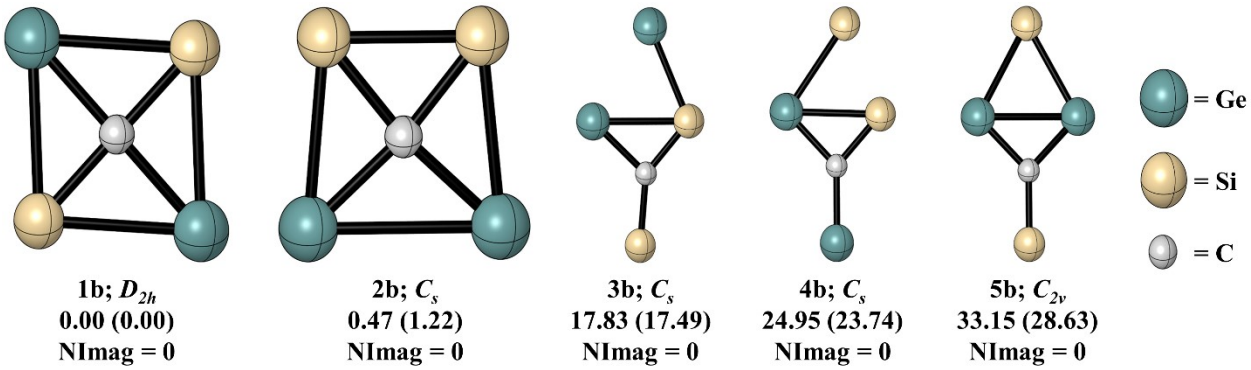

Figure S2. Low-lying isomers of $CSi_2Ge_2^{2+}$ system on the PES using PyAR program. The values without and within parentheses are the relative energies in kcal/mol at PBE0-D3(BJ)/def2-TZVP and CCSD(T)/aug-cc-pVTZ methods, respectively. The number of imaginary frequencies (NImag) obtained for each stationary point is indicated underneath the geometries.

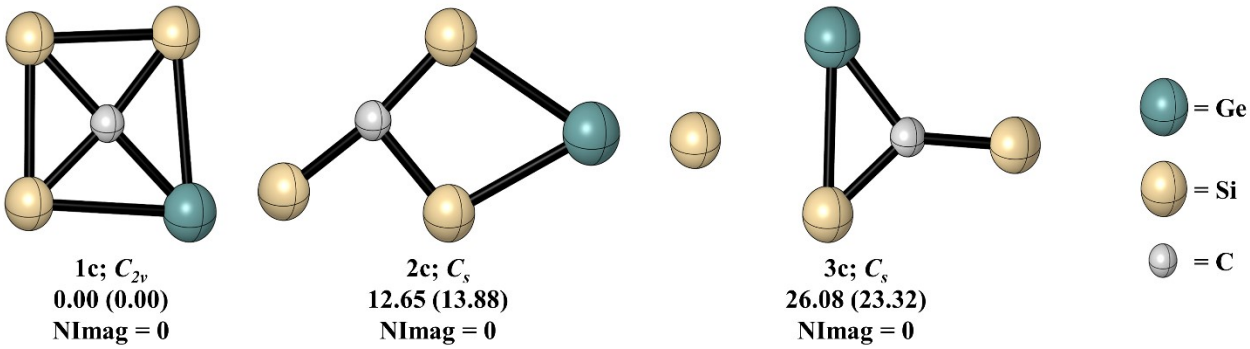

Figure S3. Low-lying isomers of CSi_3Ge^{2+} system on the PES using PyAR program. The values without and within parentheses are the relative energies in kcal/mol at PBE0-D3(BJ)/def2-TZVP and CCSD(T)/aug-cc-pVTZ methods, respectively. The number of imaginary frequencies (NImag) obtained for each stationary point is indicated underneath the geometries.

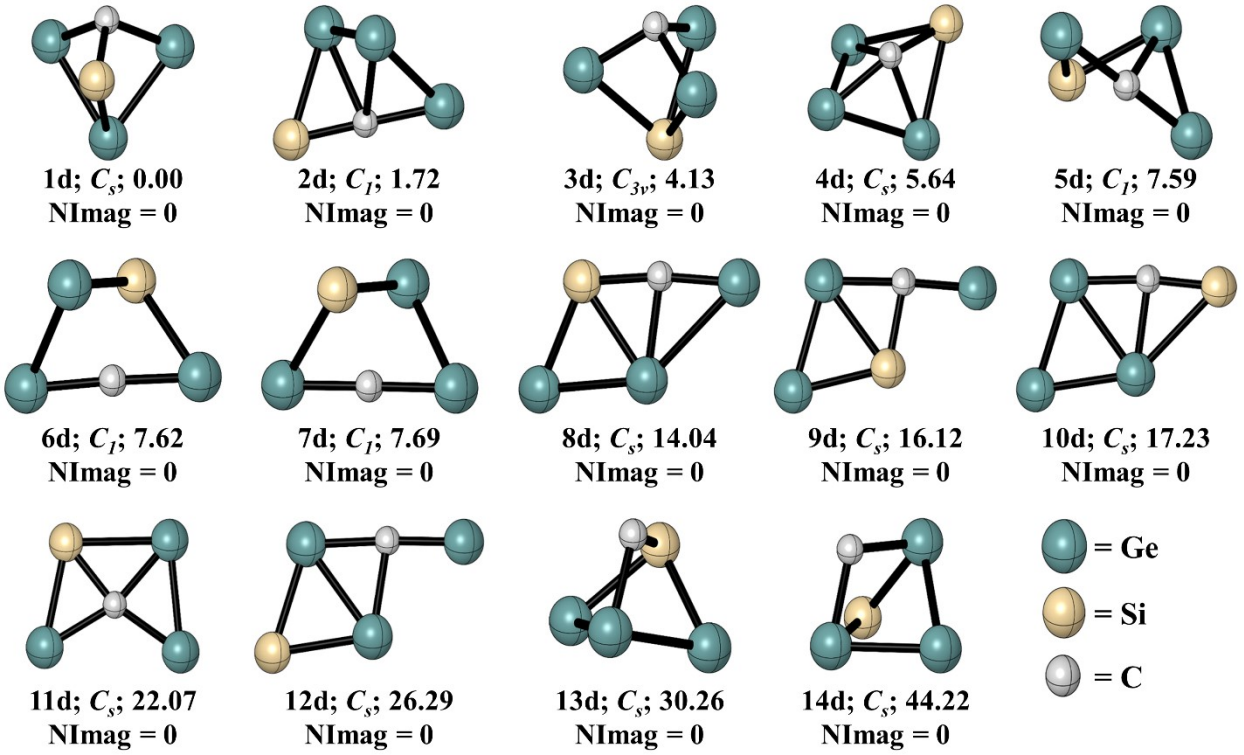

Figure S4. Low-lying isomers of $CSiGe_3$ system on the PES using ABCluster program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

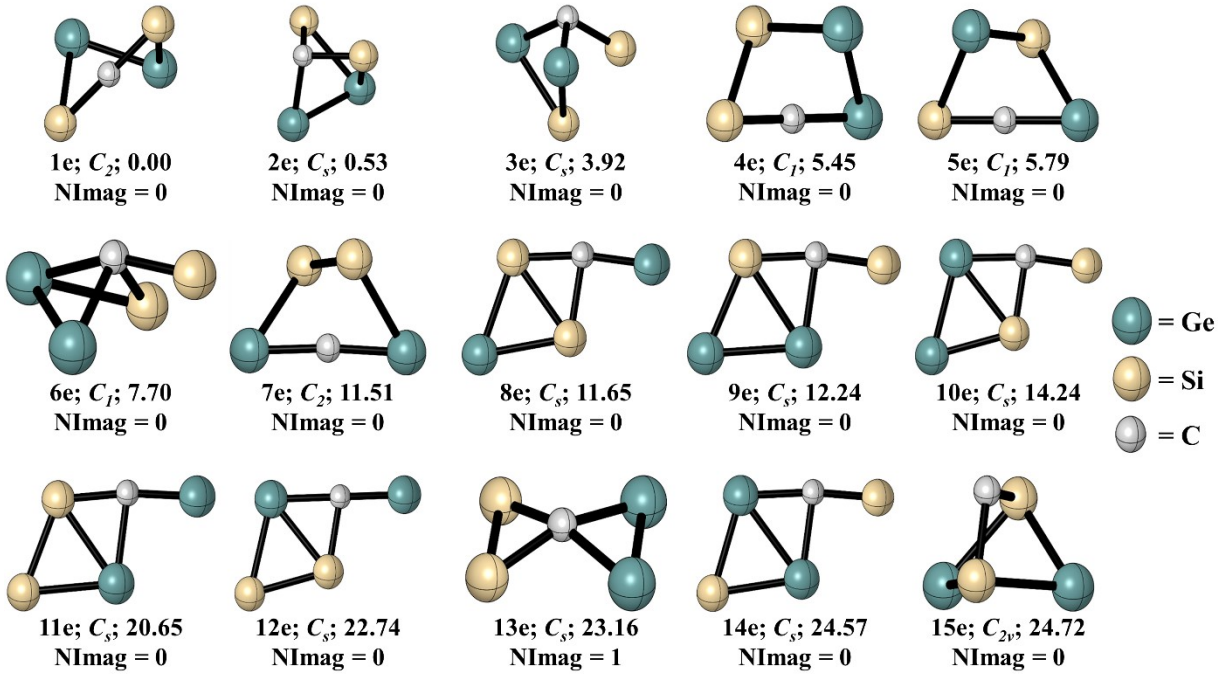

Figure S5. Low-lying isomers of CSi_2Ge_2 system on the PES using ABCluster program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

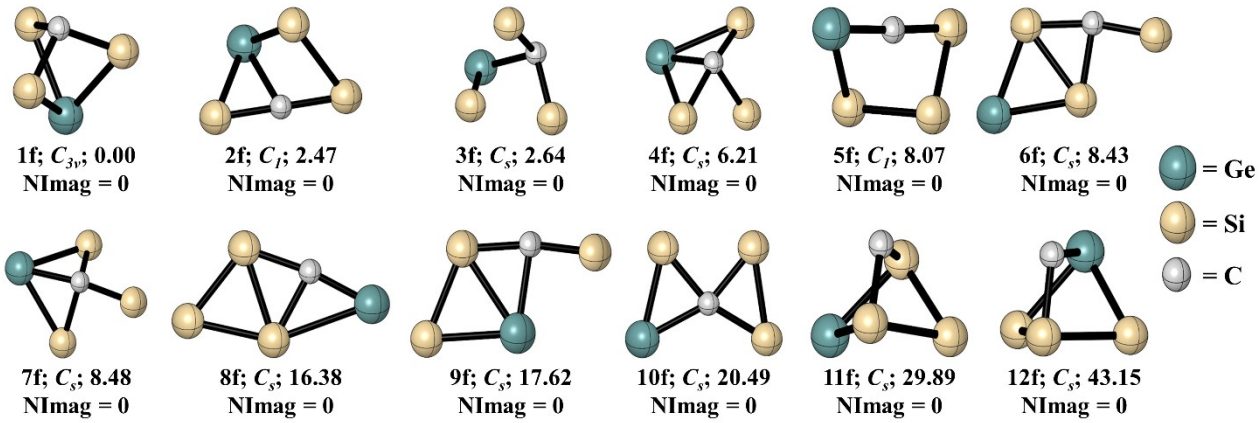

Figure S6. Low-lying isomers of CSi_3Ge system on the PES using ABCluster program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

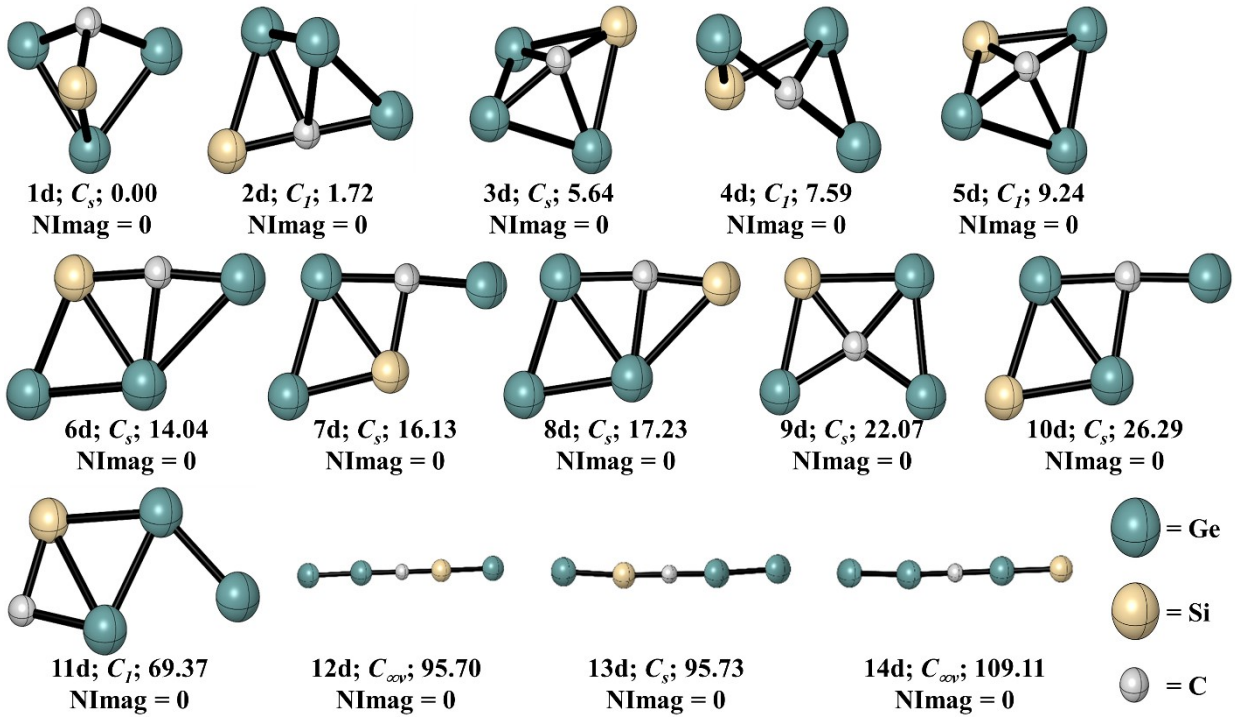

Figure S7. Low-lying isomers of $CSiGe_3$ system on the PES using PyAR program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

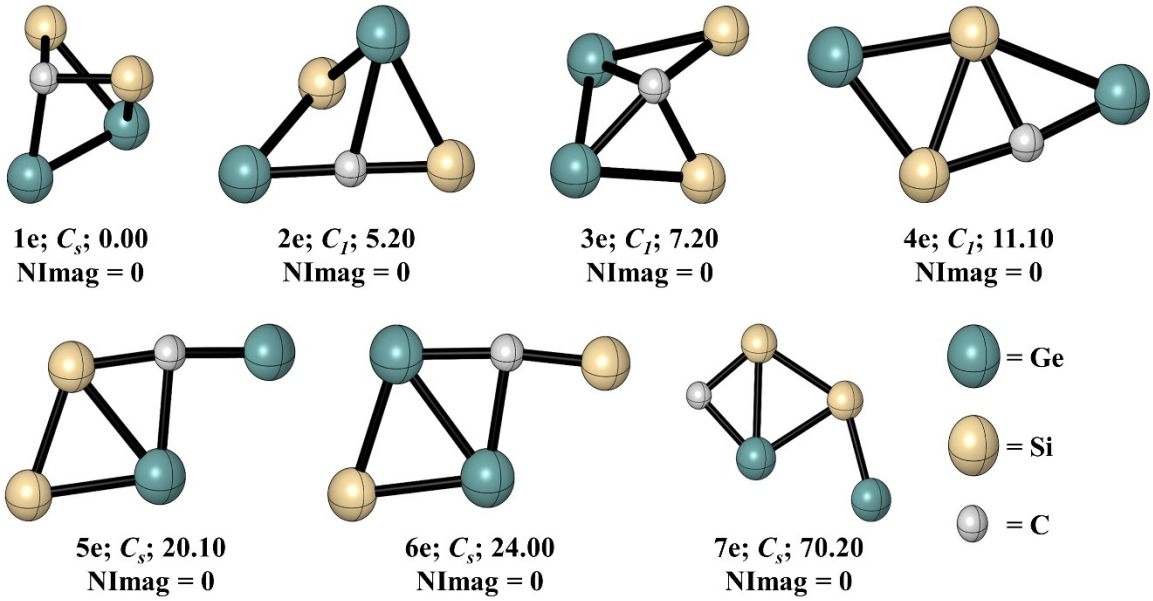

Figure S8. Low-lying isomers of CSi_2Ge_2 system on the PES using PyAR program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

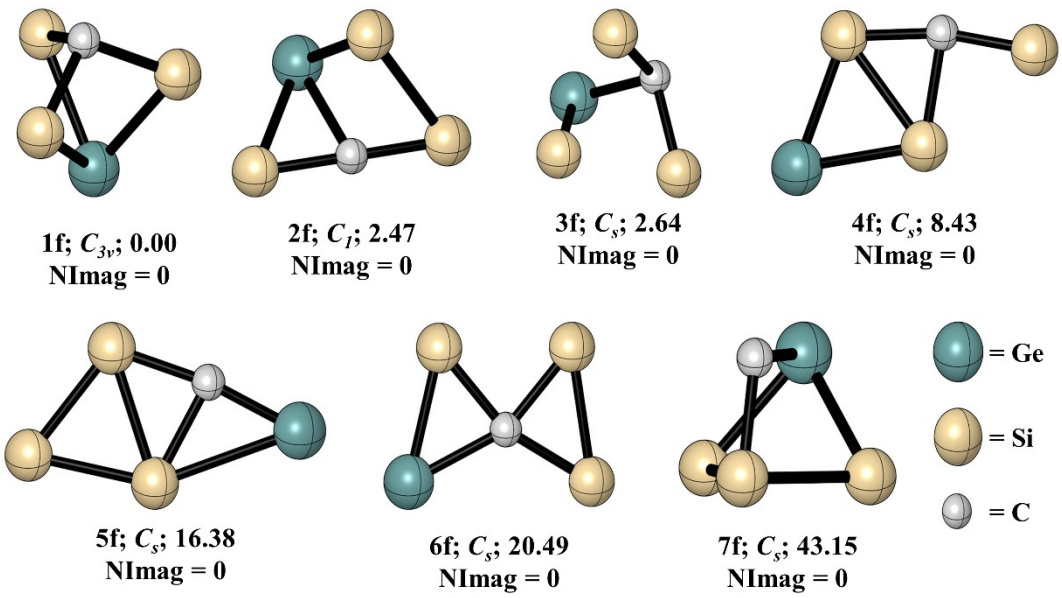

Figure S9. Low-lying isomers of CSi_3Ge system on the PES using PyAR program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

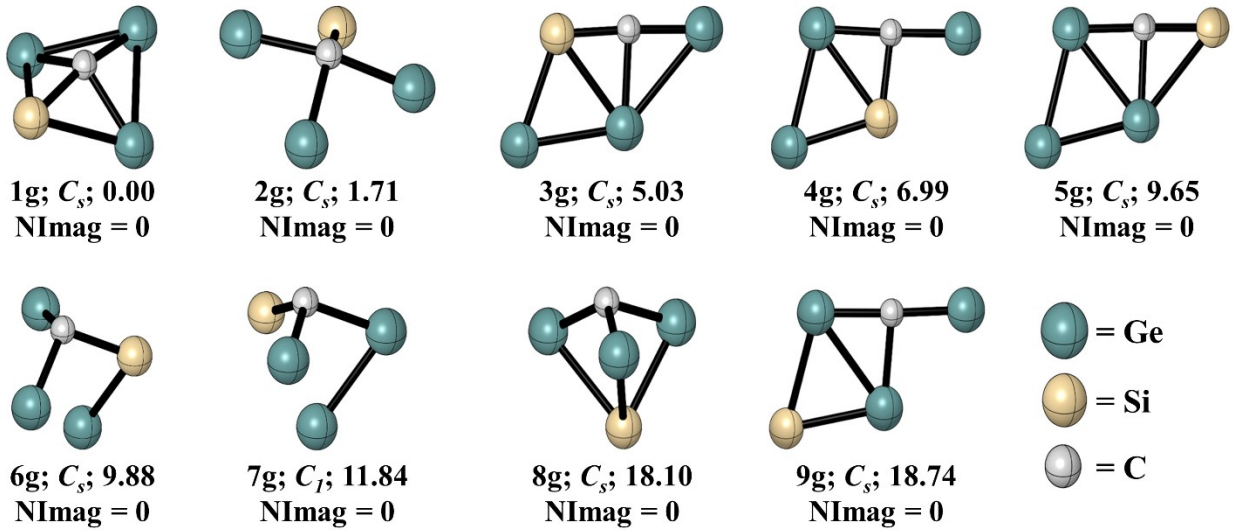

Figure S10. Low-lying isomers of $CSiGe_3^+$ system on the PES using ABCluster program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

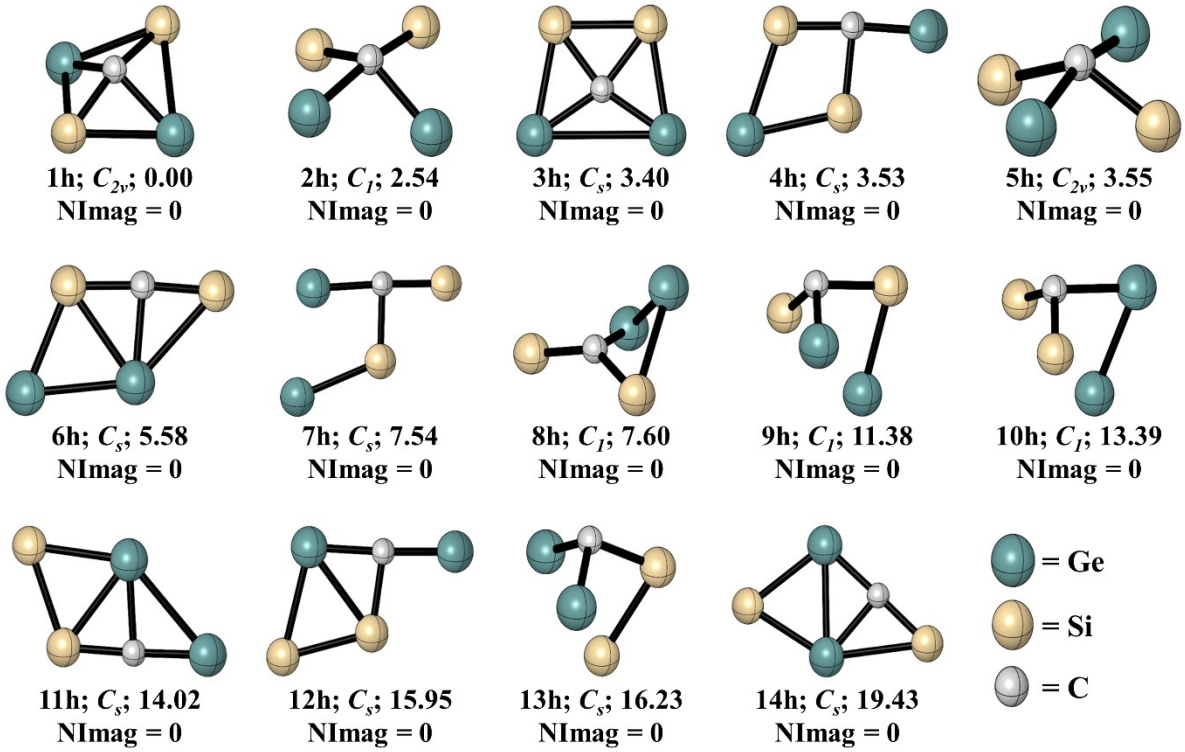

Figure S11. Low-lying isomers of $CSi_2Ge_2^+$ system on the PES using ABCluster program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

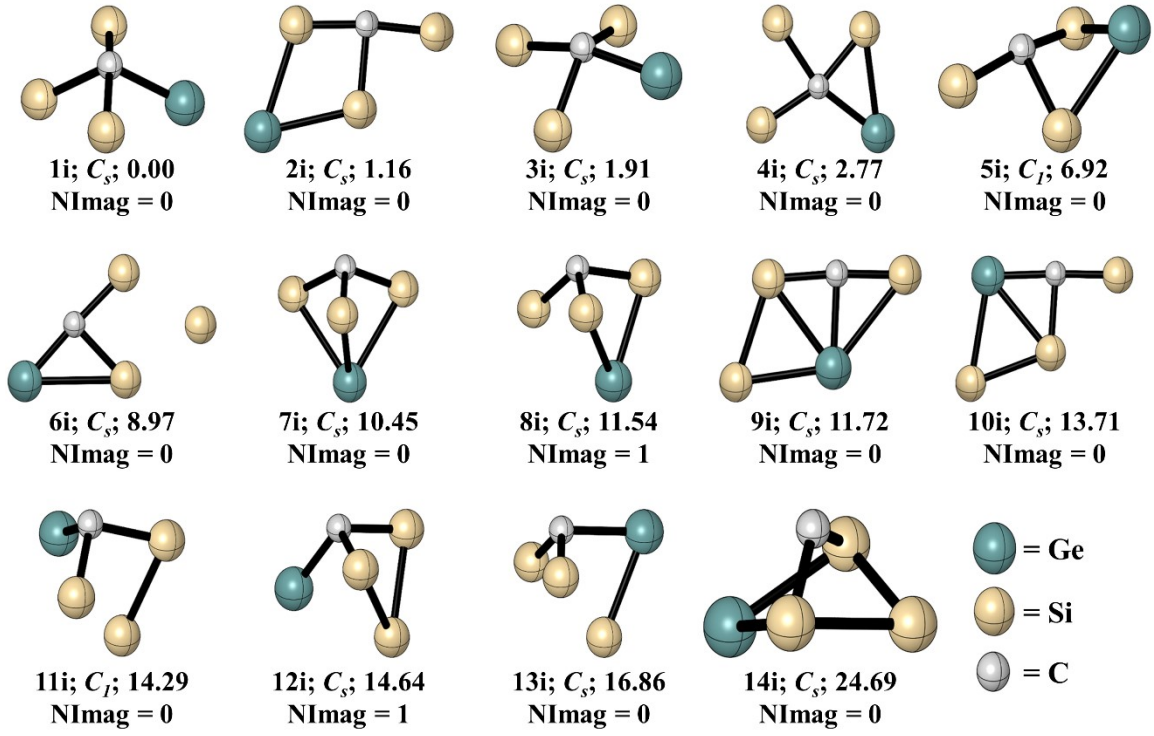

Figure S12. Low-lying isomers of CSi_3Ge^+ system on the PES using ABCluster program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

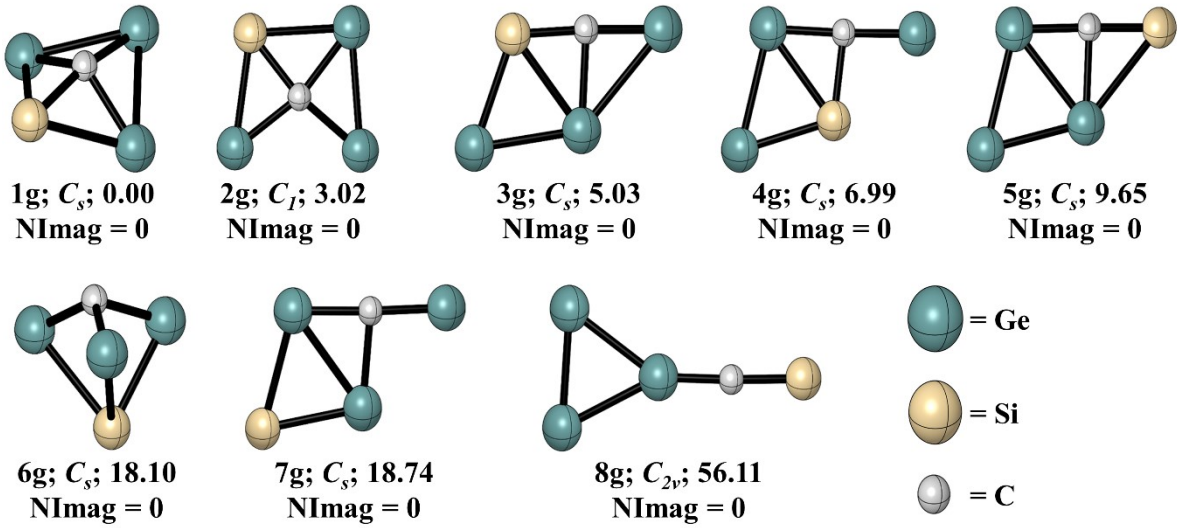

Figure S13. Low-lying isomers of $CSiGe_3^+$ system on the PES using PyAR program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

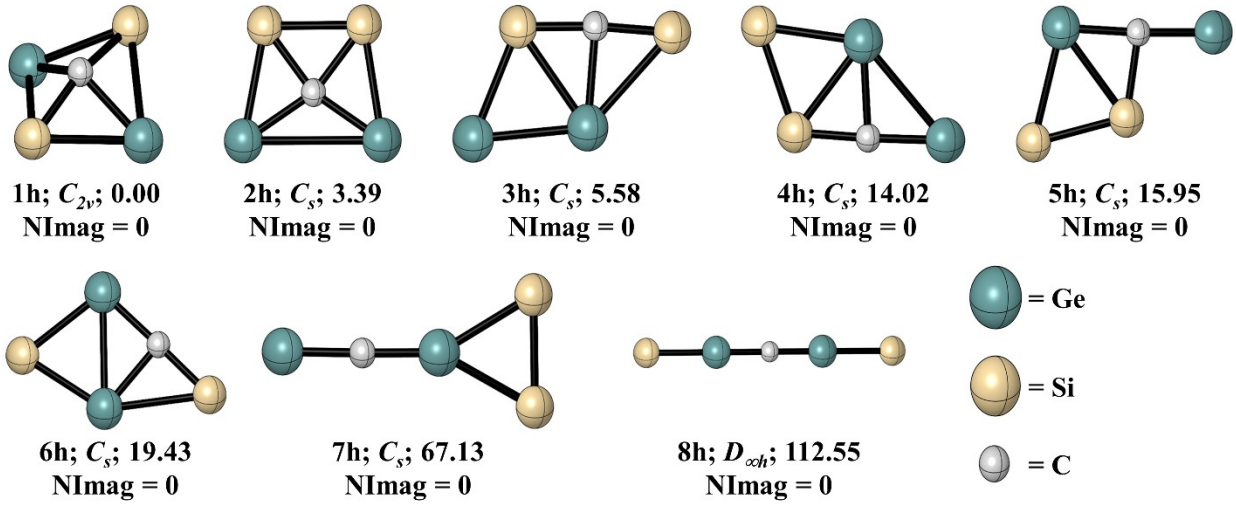

Figure S14. Low-lying isomers of $CSi_2Ge_2^+$ system on the PES using PyAR program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

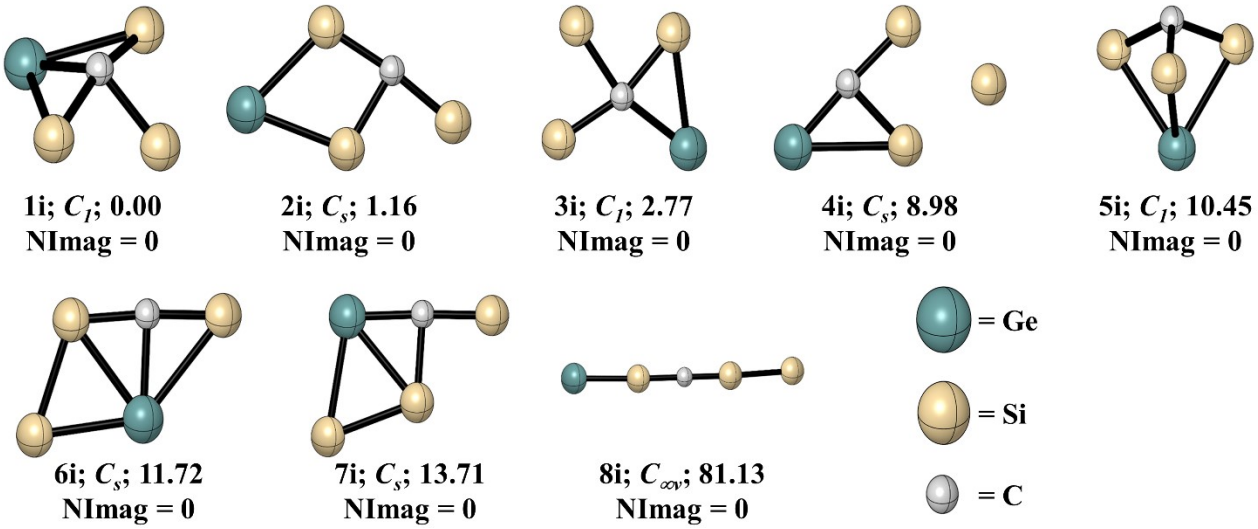

Figure S15. Low-lying isomers of CSi_3Ge^+ system on the PES using PyAR program. The relative energies are calculated at PBE0-D3(BJ)/def2-TZVP method in kcal/mol.

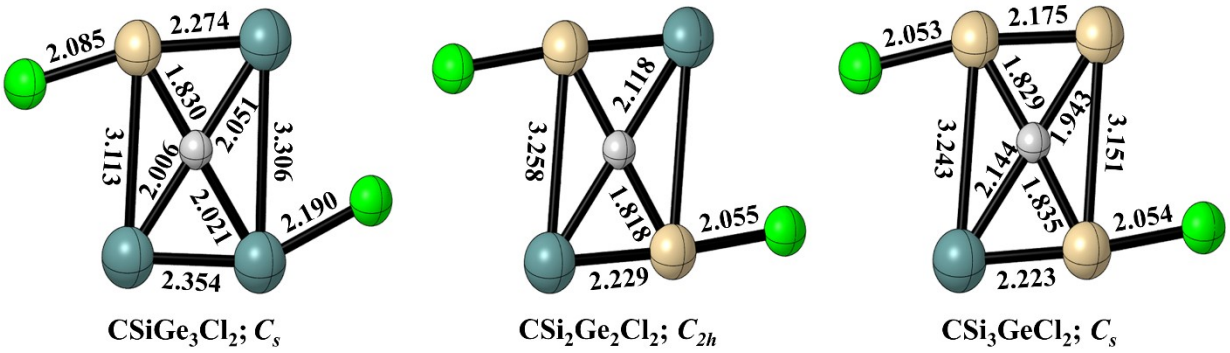

Figure S16. The optimized geometries of the $CSiGe_3Cl_2$, $CSi_2Ge_2Cl_2$, and CSi_3GeCl_2 systems. Bond lengths are given in Å unit.

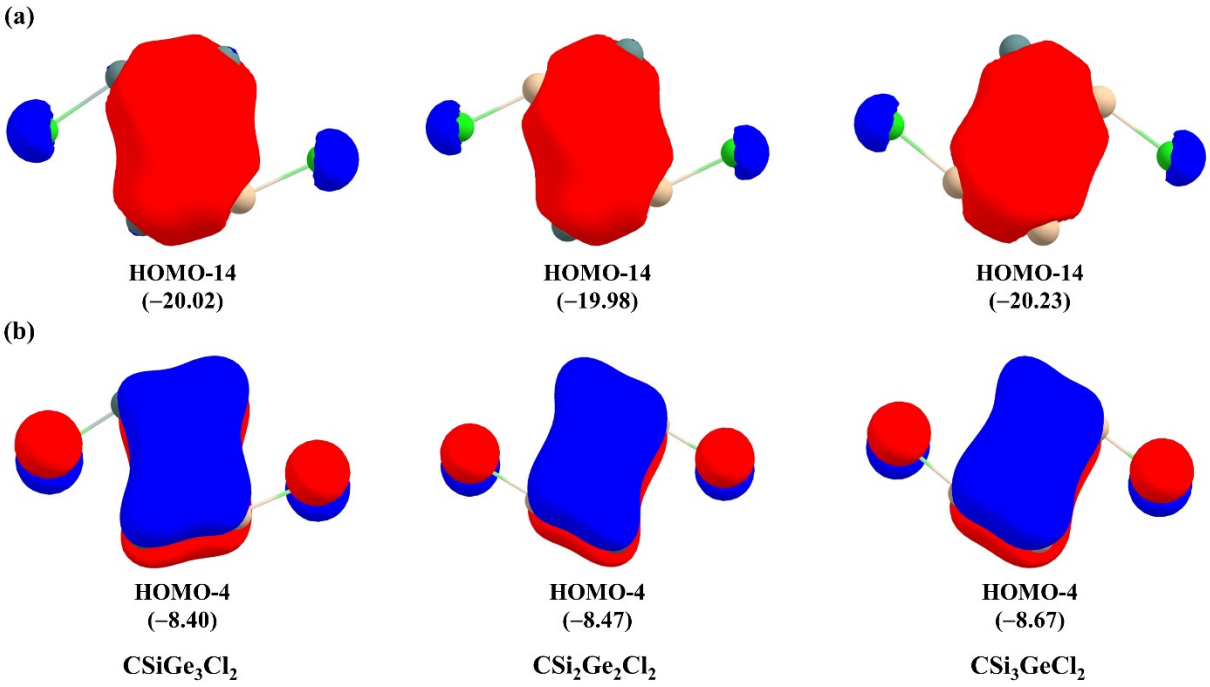

Figure S17. The (a) σ-delocalized and (b) π-delocalized molecular orbitals among the carbon and the four peripheral atoms of $CSi_nGe_{4-n}Cl_2$ (n = 1-3) systems. The values in the parenthesis are the energies of the orbitals in the eV unit.

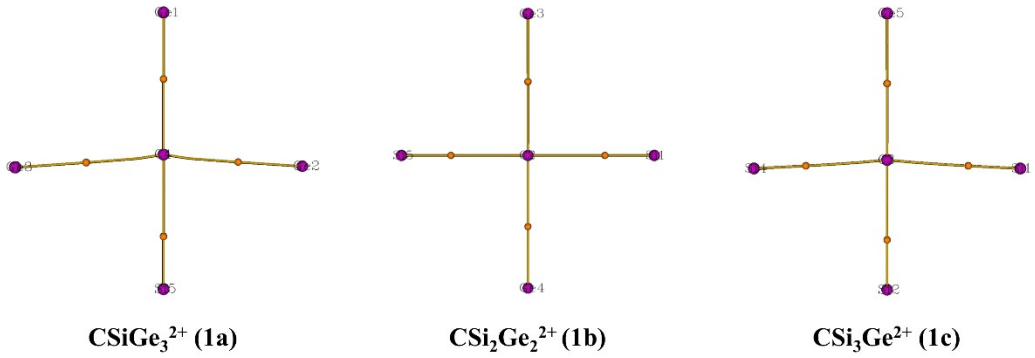

Figure S18. The plots of molecular graphs of $CSiGe_3^{2+}$ (**1a**), $CSi_2Ge_2^{2+}$ (**1b**), and CSi_3Ge^{2+} (**1c**) ptC geometries.

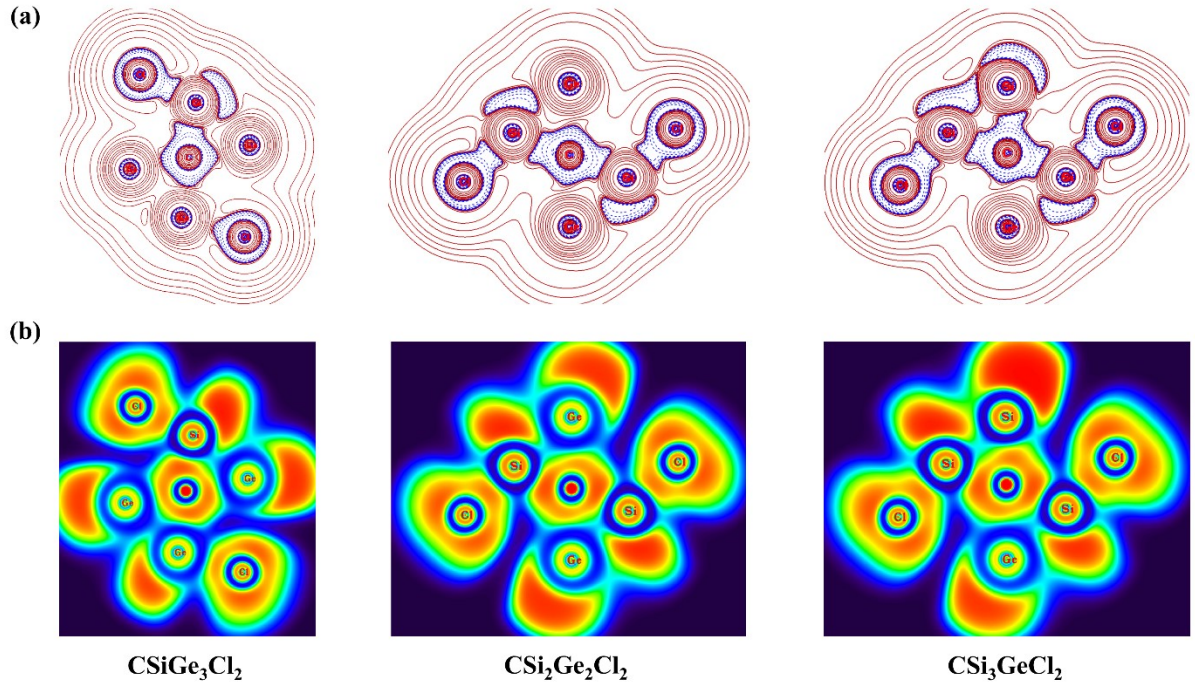

Figure S19. Plots of (a) the Laplacian of electron density [$\nabla^2\rho$(r)], blue dashed and red solid lines indicate $\nabla^2\rho$(r) < 0 and $\nabla^2\rho$(r) > 0 regions, respectively, and (b) the electron localization function (ELF) basin of $CSi_nGe_{4-n}Cl_2$ (n = 1-3) systems.

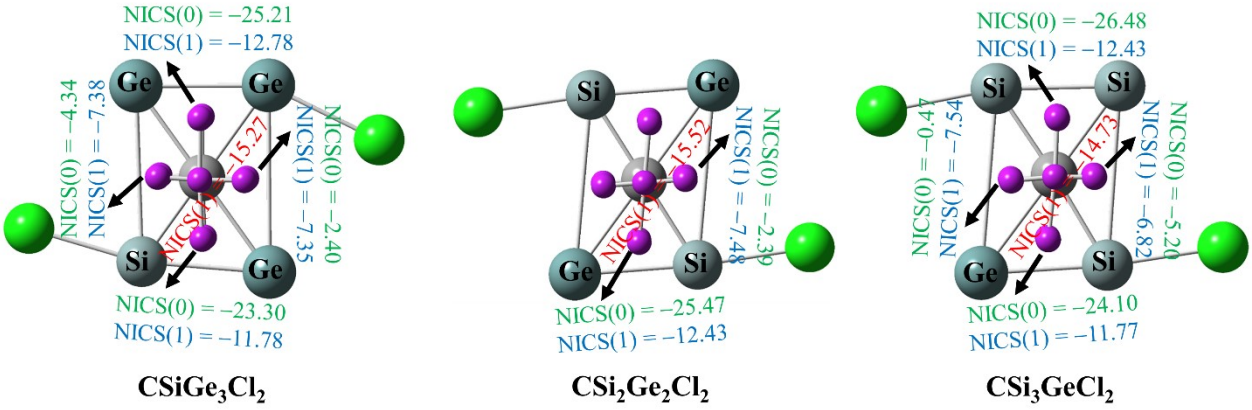

Figure S20. Nucleus independent chemical shifts (NICSs; in ppm) of $CSi_nGe_{4-n}Cl_2$ (n = 1-3) systems. The values in the red color indicate the NICS(1) values at 1 Å above the central C atom of the ring.

Table S1. The natural charges (q, $|e|$) on the atoms and the Wiberg bond indices (WBI) for C-Si and C-Ge bonds and the valence electronic configuration $CSiGe_3Cl_2$, $CSi_2Ge_2Cl_2$, and CSi_3GeCl_2 ptC structures.

Systems	q_C	q_{Si}	q_{Ge}	WBI (C-Si)	WBI (C-Ge)	Valence electronic configuration of C
$CSiGe_3Cl_2$	–1.98	0.78	0.59, 0.62, 0.69	0.80	0.58, 0.61, 0.64	$2s^{1.454}\,2p_x^{1.511}\,2p_y^{1.512}\,2p_z^{1.288}$
$CSi_2Ge_2Cl_2$	–1.92	0.78	0.50	0.80	0.53	$2s^{1.421}\,2p_x^{1.564}\,2p_y^{1.447}\,2p_z^{1.277}$
CSi_3GeCl_2	–1.95	0.57, 0.75, 0.80	0.47	0.62, 0.76,0.78	0.50	$2s^{1.419}\,2p_x^{1.558}\,2p_y^{1.483}\,2p_z^{1.277}$

Table S2. Electron Density ($\rho(r_c)$), Laplacian of Electron Density ($\nabla^2\rho(r_c)$), Kinetic Energy Density ($G(r_c)$), Potential Energy Density ($V(r_c)$), Total Energy Density ($H(r_c)$) for $CSiGe_3Cl_2$, $CSi_2Ge_2Cl_2$, and CSi_3GeCl_2 ptC structures.

Systems	BCP	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$
$CSiGe_3Cl_2$	C-Si	0.113	0.416	0.164	–0.223	–0.060
	C-Ge	0.102	0.170	0.091	–0.140	–0.049
		0.103	0.170	0.092	–0.141	–0.049
		0.095	0.160	0.083	–0.127	–0.043
$CSi_2Ge_2Cl_2$	C-Si	0.116	0.452	0.173	–0.233	–0.060
	C-Ge	0.083	0.144	0.070	–0.104	–0.034
CSi_3GeCl_2	C-Si	0.113	0.418	0.163	–0.222	–0.059
		0.113	0.438	0.167	–0.224	–0.057
		0.093	0.265	0.114	–0.162	–0.048
	C-Ge	0.078	0.147	0.067	–0.096	–0.030

Coordinates of the optimized geometries from the ABCluster program

1a			
C	0.000000000000	0.000000000000	-0.223008000000
Ge	0.000000000000	2.002416000000	-0.391058000000
Ge	0.000000000000	-2.002416000000	-0.391058000000

Ge	0.000000000000	0.000000000000	1.732085000000
Si	0.000000000000	0.000000000000	-2.075782000000
		2a	
C	0.000000000000	1.016888000000	0.000000000000
Ge	0.833420000000	-2.531636000000	0.000000000000
Ge	-0.293041000000	2.897131000000	0.000000000000
Ge	-1.164072000000	-0.541287000000	0.000000000000
Si	1.425585000000	-0.033999000000	0.000000000000
		3a	
Ge	0.000000000000	1.358367000000	-0.688633000000
Ge	0.000000000000	0.000000000000	2.549254000000
Ge	0.000000000000	-1.358367000000	-0.688633000000
C	0.000000000000	0.000000000000	0.642103000000
Si	0.000000000000	0.000000000000	-2.954019000000
		4a	
C	-0.009599000000	-1.348843000000	0.000000000000
Ge	-0.002999000000	-1.406575000000	1.914114000000
Ge	-0.002999000000	-1.406575000000	-1.914114000000
Ge	0.009110000000	2.870689000000	0.000000000000
Si	-0.002999000000	0.446560000000	0.000000000000
		5a	
C	0.000000000000	0.000000000000	0.642083000000
Ge	0.000000000000	1.358618000000	-0.688320000000
Ge	0.000000000000	0.000000000000	2.549040000000
Ge	0.000000000000	-1.358618000000	-0.688320000000
Si	0.000000000000	0.000000000000	-2.954951000000
		1b	
C	0.000000000000	0.000000000000	0.000000000000
Ge	0.000000000000	0.000000000000	2.020567000000
Ge	0.000000000000	0.000000000000	-2.020567000000
Si	0.000000000000	1.835161000000	0.000000000000
Si	0.000000000000	-1.835161000000	0.000000000000
		2b	
C	0.000000000000	-0.433143000000	0.000000000000
Ge	-1.515265000000	0.844274000000	0.000000000000
Ge	1.514784000000	0.845330000000	0.000000000000
Si	1.239090000000	-1.837367000000	0.000000000000
Si	-1.237990000000	-1.838951000000	0.000000000000
		3b	

C	0.000000000000	0.000000000000	0.908134000000
Ge	0.000000000000	0.000000000000	2.819691000000
Ge	0.000000000000	0.000000000000	-2.666945000000
Si	0.000000000000	1.272578000000	-0.369168000000
Si	0.000000000000	-1.272578000000	-0.369168000000
		4b	
C	1.569290000000	0.055568000000	0.000000000000
Ge	-1.982612000000	-0.821912000000	0.000000000000
Ge	0.000000000000	1.218572000000	0.000000000000
Si	0.541500000000	-1.384229000000	0.000000000000
Si	3.317631000000	0.453763000000	0.000000000000
		5b	
C	0.000000000000	0.561640000000	0.000000000000
Ge	-0.783285000000	2.304856000000	0.000000000000
Ge	-0.688671000000	-1.260135000000	0.000000000000
Si	1.713120000000	-2.550291000000	0.000000000000
Si	1.651351000000	-0.078347000000	0.000000000000
		6b	
C	0.000000000000	0.000000000000	1.122541000000
Ge	0.000000000000	1.370206000000	-0.198882000000
Ge	0.000000000000	-1.370206000000	-0.198882000000
Si	0.000000000000	0.000000000000	2.918304000000
Si	0.000000000000	0.000000000000	-2.490216000000
		1c	
C	0.000000000000	0.000000000000	-0.427360000000
Ge	0.000000000000	0.000000000000	1.569770000000
Si	0.000000000000	1.851175000000	-0.546265000000
Si	0.000000000000	-1.851175000000	-0.546265000000
Si	0.000000000000	0.000000000000	-2.312363000000
		2c	
Si	0.000000000000	1.136138000000	0.000000000000
Si	0.805783000000	-1.308498000000	0.000000000000
C	1.616002000000	0.261150000000	0.000000000000
Si	2.667849000000	1.724412000000	0.000000000000
Ge	-1.822714000000	-0.727988000000	0.000000000000
		3c	
C	0.000000000000	0.000000000000	-1.565604000000
Ge	0.000000000000	0.000000000000	2.023021000000

Si	0.000000000000	0.000000000000	-3.366170000000
Si	0.000000000000	1.281560000000	-0.293453000000
Si	0.000000000000	-1.281560000000	-0.293453000000
		4c	
C	0.000000000000	0.000000000000	0.291139000000
Ge	0.000000000000	0.000000000000	2.211472000000
Si	0.000000000000	1.262745000000	-0.996164000000
Si	0.000000000000	0.000000000000	-3.187238000000
Si	0.000000000000	-1.262745000000	-0.996164000000
		5c	
C	0.000000000000	1.115924000000	0.000000000000
Ge	-0.982202000000	-0.575405000000	0.000000000000
Si	1.532608000000	0.232025000000	0.000000000000
Si	-0.516162000000	2.839758000000	0.000000000000
Si	1.228587000000	-2.234826000000	0.000000000000
		6c	
C	0.143758000000	0.461628000000	0.000000000000
Ge	-0.456245000000	-1.484641000000	0.000000000000
Si	-0.456245000000	1.701032000000	1.281358000000
Si	1.893726000000	-0.206440000000	0.000000000000
Si	-0.456245000000	1.701032000000	-1.281358000000
		1d	
C	1.260968000000	0.316828000000	0.000000000000
Ge	-1.346035000000	0.267527000000	0.000000000000
Ge	0.455222000000	-0.589202000000	1.515459000000
Ge	0.455222000000	-0.589202000000	-1.515459000000
Si	0.455222000000	1.946222000000	0.000000000000
		2d	
C	-0.093798000000	0.991295000000	0.411027000000
Ge	-1.760085000000	0.594560000000	-0.327433000000
Ge	-0.301395000000	-1.246566000000	0.542665000000
Ge	1.437216000000	-0.145095000000	-0.780133000000
Si	1.467088000000	1.397106000000	1.115049000000
		3d	
C	0.000000000000	0.000000000000	-1.004464000000
Ge	0.000000000000	1.744490000000	-0.162311000000
Ge	-1.510772000000	-0.872245000000	-0.162311000000
Ge	1.510772000000	-0.872245000000	-0.162311000000
Si	0.000000000000	0.000000000000	1.543471000000

	4d		
C	0.312285000000	0.890596000000	0.000000000000
Ge	0.312285000000	-0.388837000000	1.564514000000
Ge	0.312285000000	-0.388837000000	-1.564514000000
Ge	-1.593622000000	0.239880000000	0.000000000000
Si	2.081140000000	0.847558000000	0.000000000000
	5d		
C	0.244490000000	0.688154000000	-0.088044000000
Ge	-1.565194000000	1.090304000000	0.080762000000
Ge	2.073208000000	0.388519000000	-0.285818000000
Ge	-0.852187000000	-1.281482000000	-0.372808000000
Si	0.681900000000	-0.745988000000	1.358566000000
	6d		
C	0.252758000000	-0.685055000000	0.119108000000
Ge	-0.868546000000	1.280471000000	0.367094000000
Ge	2.082492000000	-0.372590000000	0.282685000000
Ge	-1.552859000000	-1.099450000000	-0.077666000000
Si	0.666334000000	0.731469000000	-1.358733000000
	7d		
C	-0.235262000000	-0.729846000000	-0.080995000000
Ge	1.590933000000	-1.059556000000	0.070534000000
Ge	0.811307000000	1.286584000000	-0.369616000000
Ge	-2.059852000000	-0.397793000000	-0.289059000000
Si	-0.681775000000	0.703112000000	1.379036000000
	8d		
C	0.918961000000	-0.974473000000	0.000000000000
Ge	2.580635000000	-0.288981000000	0.000000000000
Ge	0.000000000000	0.846539000000	0.000000000000
Ge	-2.400381000000	0.254757000000	0.000000000000
Si	-0.805850000000	-1.439090000000	0.000000000000
	9d		
C	1.124041000000	-0.453625000000	0.000000000000
Ge	-2.282745000000	0.494707000000	0.000000000000
Ge	-0.611829000000	-1.303555000000	0.000000000000
Ge	2.683816000000	0.441372000000	0.000000000000
Si	0.000000000000	1.034357000000	0.000000000000
	10d		
C	1.679819000000	-0.043522000000	0.000000000000
Ge	0.000000000000	-1.144147000000	0.000000000000

Ge	0.372656000000	1.341587000000	0.000000000000
Ge	-1.871264000000	0.426752000000	0.000000000000
Si	2.705468000000	-1.408073000000	0.000000000000
		11d	
C	0.000000000000	0.206381000000	0.000000000000
Ge	0.708826000000	2.048462000000	0.000000000000
Ge	1.197743000000	-1.313383000000	0.000000000000
Ge	-1.249612000000	-1.322897000000	0.000000000000
Si	-1.501614000000	1.255136000000	0.000000000000
		12d	
C	0.000000000000	-0.958516000000	0.000000000000
Ge	-1.666091000000	-0.026335000000	0.000000000000
Ge	0.627750000000	0.946932000000	0.000000000000
Ge	1.610109000000	-1.749512000000	0.000000000000
Si	-1.306897000000	2.305458000000	0.000000000000
		13d	
C	-1.520653000000	0.760598000000	0.000000000000
Ge	0.298972000000	1.364318000000	0.000000000000
Ge	0.298972000000	-0.525863000000	1.579349000000
Ge	0.298972000000	-0.525863000000	-1.579349000000
Si	-1.398383000000	-1.040468000000	0.000000000000
		14d	
C	1.135716000000	-1.086273000000	0.000000000000
Ge	0.155981000000	-0.414543000000	1.502271000000
Ge	0.155981000000	1.515113000000	0.000000000000
Ge	0.155981000000	-0.414543000000	-1.502271000000
Si	-1.556317000000	-1.102518000000	0.000000000000
		1e	
C	0.000000000000	0.000000000000	1.234307000000
Ge	0.000000000000	1.223500000000	-0.654307000000
Ge	0.000000000000	-1.223500000000	-0.654307000000
Si	1.509472000000	-0.916546000000	1.231064000000
Si	-1.509472000000	0.916546000000	1.231064000000
		2e	
C	1.334694000000	0.369512000000	0.000000000000
Ge	-1.259111000000	0.318169000000	0.000000000000
Ge	0.538056000000	-1.409926000000	0.000000000000
Si	0.538056000000	1.168541000000	1.433101000000
Si	0.538056000000	1.168541000000	-1.433101000000

	3e		
C	0.505998000000	0.958902000000	0.000000000000
Ge	0.505998000000	-0.266542000000	1.509466000000
Ge	0.505998000000	-0.266542000000	-1.509466000000
Si	-1.202679000000	1.593251000000	0.000000000000
Si	-1.327311000000	-0.785731000000	0.000000000000
	4e		
C	-0.342580000000	0.922904000000	-0.287549000000
Ge	0.081043000000	-1.317612000000	-0.286019000000
Ge	1.475136000000	0.727456000000	0.093210000000
Si	-1.350518000000	-0.154505000000	1.209945000000
Si	-2.059643000000	1.107900000000	-0.646004000000
	5e		
C	0.208735000000	0.903056000000	-0.024549000000
Ge	-1.407152000000	-0.663037000000	-0.386828000000
Ge	1.855322000000	0.052929000000	-0.292226000000
Si	-1.339697000000	1.702504000000	0.227170000000
Si	0.225850000000	-0.694994000000	1.335473000000
	6e		
C	-0.379140000000	0.500088000000	-0.705295000000
Ge	1.551693000000	0.091654000000	-0.219693000000
Ge	-0.534595000000	-1.275932000000	0.231222000000
Si	-2.107154000000	0.811616000000	-0.468978000000
Si	-0.055155000000	1.680982000000	0.744895000000
	7e		
C	0.000000000000	0.000000000000	0.459920000000
Ge	0.000000000000	1.862413000000	0.530790000000
Ge	0.000000000000	-1.862413000000	0.530790000000
Si	-0.980620000000	0.599052000000	-1.311789000000
Si	0.980620000000	-0.599052000000	-1.311789000000
	8e		
C	0.903355000000	-0.830794000000	0.000000000000
Ge	-2.343116000000	0.442734000000	0.000000000000
Ge	2.534497000000	-0.059816000000	0.000000000000
Si	-0.824595000000	-1.348967000000	0.000000000000
Si	0.000000000000	0.829778000000	0.000000000000
	9e		
C	1.738512000000	-0.133160000000	0.000000000000
Ge	-1.726005000000	-0.841505000000	0.000000000000

Ge	0.000000000000	0.931693000000	0.000000000000
Si	0.517689000000	-1.440689000000	0.000000000000
Si	2.682389000000	1.291615000000	0.000000000000
		10e	
C	-1.644723000000	0.339135000000	0.000000000000
Ge	1.841815000000	-0.231197000000	0.000000000000
Ge	-0.427262000000	-1.157505000000	0.000000000000
Si	0.000000000000	1.225438000000	0.000000000000
Si	-2.528382000000	1.803393000000	0.000000000000
		11e	
C	0.001400000000	-1.033619000000	0.000000000000
Ge	-1.785949000000	-1.204170000000	0.000000000000
Ge	0.000000000000	1.009887000000	0.000000000000
Si	1.747444000000	-0.646729000000	0.000000000000
Si	2.334126000000	1.533784000000	0.000000000000
		12e	
C	0.000000000000	0.777332000000	0.000000000000
Ge	-1.477922000000	1.798057000000	0.000000000000
Ge	1.538781000000	-0.401713000000	0.000000000000
Si	0.670339000000	-2.622965000000	0.000000000000
Si	-0.809445000000	-0.901819000000	0.000000000000
		13e	
C	0.316073000000	0.580514000000	0.000000000000
Ge	-0.020613000000	-0.915260000000	1.228637000000
Ge	-0.020613000000	-0.915260000000	-1.228637000000
Si	-0.020613000000	1.967628000000	-1.155327000000
Si	-0.020613000000	1.967628000000	1.155327000000
		14e	
C	1.249913000000	-0.460637000000	0.000000000000
Ge	-0.440080000000	-1.343283000000	0.000000000000
Ge	0.000000000000	1.113995000000	0.000000000000
Si	-2.194196000000	0.228325000000	0.000000000000
Si	2.664417000000	0.493178000000	0.000000000000
		15e	
C	0.000000000000	0.000000000000	1.751109000000
Ge	0.000000000000	1.560253000000	-0.449585000000
Ge	0.000000000000	-1.560253000000	-0.449585000000
Si	1.434431000000	0.000000000000	0.652385000000
Si	-1.434431000000	0.000000000000	0.652385000000

	1f		
C	0.000000000000	0.000000000000	-1.449493000000
Ge	0.000000000000	0.000000000000	1.136421000000
Si	0.000000000000	1.652521000000	-0.658774000000
Si	1.431125000000	-0.826260000000	-0.658774000000
Si	-1.431125000000	-0.826260000000	-0.658774000000
	2f		
C	0.588620000000	0.921342000000	-0.193082000000
Ge	-1.008894000000	-0.684819000000	-0.304706000000
Si	2.117911000000	0.160888000000	-0.656384000000
Si	0.869659000000	-0.670760000000	1.151549000000
Si	-0.933791000000	1.680311000000	0.284055000000
	3f		
C	-1.056436000000	-0.436956000000	0.000000000000
Ge	-0.235458000000	1.334108000000	0.000000000000
Si	-0.235458000000	-1.234800000000	1.427081000000
Si	1.461865000000	-0.392523000000	0.000000000000
Si	-0.235458000000	-1.234800000000	-1.427081000000
	4f		
C	0.423951000000	0.810756000000	0.000000000000
Ge	-1.236290000000	-0.329140000000	0.000000000000
Si	0.423951000000	0.456292000000	1.796841000000
Si	0.423951000000	0.456292000000	-1.796841000000
Si	1.796211000000	-0.507731000000	0.000000000000
	5f		
C	0.287085000000	-0.677008000000	0.124959000000
Ge	-1.527615000000	-0.319828000000	-0.148373000000
Si	-0.004105000000	1.299906000000	0.831650000000
Si	1.984222000000	-1.076216000000	0.383087000000
Si	1.388536000000	0.797491000000	-0.929153000000
	6f		
C	1.705661000000	0.193851000000	0.000000000000
Ge	-1.663268000000	-0.692304000000	0.000000000000
Si	0.000000000000	1.007509000000	0.000000000000
Si	2.456509000000	1.735455000000	0.000000000000
Si	0.614248000000	-1.243634000000	0.000000000000

	7f		
C	-0.805059000000	0.273872000000	0.000000000000
Ge	0.347911000000	-1.414766000000	0.000000000000
Si	0.347911000000	0.548265000000	1.472635000000
Si	-1.146021000000	2.019848000000	0.000000000000
Si	0.347911000000	0.548265000000	-1.472635000000
	8f		
C	0.000000000000	0.806235000000	0.000000000000
Ge	-1.799954000000	0.878988000000	0.000000000000
Si	0.069453000000	-1.085359000000	0.000000000000
Si	1.776386000000	0.477203000000	0.000000000000
Si	2.268342000000	-1.746488000000	0.000000000000
	9f		
C	1.017206000000	-0.933560000000	0.000000000000
Ge	0.000000000000	0.838319000000	0.000000000000
Si	-2.285345000000	0.116446000000	0.000000000000
Si	2.538550000000	-0.158889000000	0.000000000000
Si	-0.689150000000	-1.473618000000	0.000000000000
	10f		
C	0.000000000000	0.442548000000	0.000000000000
Ge	-0.782672000000	-1.402312000000	0.000000000000
Si	-0.966402000000	1.988811000000	0.000000000000
Si	1.316903000000	1.746346000000	0.000000000000
Si	1.438464000000	-0.719536000000	0.000000000000
	11f		
C	1.556484000000	0.644123000000	0.000000000000
Ge	-1.147221000000	0.650903000000	0.000000000000
Si	0.651718000000	0.018446000000	1.432822000000
Si	0.651718000000	-1.800722000000	0.000000000000
Si	0.651718000000	0.018446000000	-1.432822000000
	12f		
C	1.385920000000	0.489208000000	0.000000000000
Ge	-0.423374000000	1.124704000000	0.000000000000
Si	1.220496000000	-1.308908000000	0.000000000000
Si	-0.423374000000	-0.735752000000	1.499800000000
Si	-0.423374000000	-0.735752000000	-1.499800000000
	1g		
C	0.317246000000	0.564287000000	0.000000000000
Ge	0.317246000000	-0.335670000000	1.780744000000

Ge	0.317246000000	-0.335670000000	-1.780744000000
Ge	-1.615171000000	0.509772000000	0.000000000000
Si	2.105591000000	0.127460000000	0.000000000000
		2g	
C	0.360911000000	0.370566000000	0.000000000000
Ge	-1.568080000000	0.073513000000	0.000000000000
Ge	0.360911000000	0.105276000000	1.956808000000
Ge	0.360911000000	0.105276000000	-1.956808000000
Si	1.779626000000	-0.808105000000	0.000000000000
		3g	
C	0.930445000000	-0.900252000000	0.000000000000
Ge	-2.478920000000	0.115747000000	0.000000000000
Ge	2.611047000000	-0.141940000000	0.000000000000
Ge	0.000000000000	0.872440000000	0.000000000000
Si	-0.700767000000	-1.548457000000	0.000000000000
		4g	
C	1.085052000000	-0.413490000000	0.000000000000
Ge	-2.359092000000	0.508671000000	0.000000000000
Ge	2.697073000000	0.479356000000	0.000000000000
Ge	-0.541429000000	-1.380770000000	0.000000000000
Si	0.000000000000	1.074909000000	0.000000000000
		5g	
C	-1.624748000000	0.072356000000	0.000000000000
Ge	-0.462782000000	-1.390521000000	0.000000000000
Ge	1.938558000000	-0.457780000000	0.000000000000
Ge	0.000000000000	1.195035000000	0.000000000000
Si	-2.676882000000	1.462172000000	0.000000000000
		6g	
C	-1.234394000000	0.105739000000	0.000000000000
Ge	-0.495767000000	-0.597192000000	1.624940000000
Ge	1.439880000000	0.393610000000	0.000000000000
Ge	-0.495767000000	-0.597192000000	-1.624940000000
Si	-0.495767000000	1.785021000000	0.000000000000
		7g	
C	-0.313489000000	-0.635453000000	1.023683000000
Ge	1.164945000000	-1.115133000000	-0.229103000000
Ge	-1.763893000000	-0.309508000000	-0.161275000000
Ge	0.476218000000	1.227516000000	-0.647785000000
Si	0.414878000000	0.722907000000	1.934222000000

	8g		
C	0.738061000000	0.510932000000	0.000000000000
Ge	-1.073602000000	1.318748000000	0.000000000000
Ge	0.738061000000	-0.468568000000	1.633490000000
Ge	0.738061000000	-0.468568000000	-1.633490000000
Si	-1.236358000000	-1.091226000000	0.000000000000
	9g		
C	0.000000000000	0.894021000000	0.000000000000
Ge	-1.647568000000	1.713253000000	0.000000000000
Ge	1.703442000000	0.114252000000	0.000000000000
Ge	-0.653466000000	-0.964144000000	0.000000000000
Si	1.365926000000	-2.356549000000	0.000000000000
	1h		
C	0.000000000000	0.000000000000	0.724742000000
Ge	0.000000000000	1.765103000000	-0.248666000000
Ge	0.000000000000	-1.765103000000	-0.248666000000
Si	1.794541000000	0.000000000000	0.413078000000
Si	-1.794541000000	0.000000000000	0.413078000000
	2h		
C	-0.076626000000	0.444201000000	-0.506621000000
Ge	-1.114199000000	-1.096347000000	0.163877000000
Ge	1.622989000000	-0.418388000000	-0.116044000000
Si	-1.689786000000	1.358826000000	-0.342693000000
Si	0.559676000000	1.913054000000	0.450483000000
	3h		
C	0.001426000000	0.256576000000	0.000000000000
Ge	-0.000093000000	-0.753756000000	1.687411000000
Ge	-0.000093000000	-0.753756000000	-1.687411000000
Si	-0.000093000000	1.667890000000	1.207916000000
Si	-0.000093000000	1.667890000000	-1.207916000000
	4h		
C	0.906603000000	-0.772840000000	0.000000000000
Ge	2.567648000000	0.046269000000	0.000000000000
Ge	-2.419531000000	0.356703000000	0.000000000000
Si	0.000000000000	0.859103000000	0.000000000000
Si	-0.727098000000	-1.448964000000	0.000000000000
	5h		
C	0.000000000000	0.000000000000	0.419721000000
Ge	0.000000000000	1.967782000000	0.100199000000

Ge	0.000000000000	-1.967782000000	0.100199000000
Si	1.671798000000	0.000000000000	-0.318967000000
Si	-1.671798000000	0.000000000000	-0.318967000000
		6h	
C	1.697252000000	-0.076952000000	0.000000000000
Ge	-1.751327000000	-0.940103000000	0.000000000000
Ge	0.000000000000	0.990175000000	0.000000000000
Si	0.623642000000	-1.466570000000	0.000000000000
Si	2.651998000000	1.385098000000	0.000000000000
		7h	
C	1.597766000000	0.344052000000	0.000000000000
Ge	-1.922639000000	-0.213308000000	0.000000000000
Ge	0.516869000000	-1.204419000000	0.000000000000
Si	2.528433000000	1.821999000000	0.000000000000
Si	0.000000000000	1.271069000000	0.000000000000
		8h	
C	-0.223485000000	0.922240000000	-0.193088000000
Ge	1.375769000000	-0.509398000000	-0.391361000000
Ge	-0.995983000000	-0.926661000000	0.388463000000
Si	1.149107000000	1.670098000000	0.738724000000
Si	-1.921411000000	1.217075000000	-0.649347000000
		9h	
C	0.425365000000	-1.258837000000	0.263524000000
Ge	1.601414000000	0.212441000000	-0.120211000000
Ge	-1.039928000000	0.934238000000	-0.216984000000
Si	-0.872650000000	-1.566931000000	-0.952469000000
Si	-0.593046000000	-0.514550000000	1.610262000000
		10h	
C	-0.125271000000	1.356731000000	0.002698000000
Ge	0.853486000000	-1.050867000000	-0.002533000000
Ge	-1.448257000000	-0.169849000000	0.001653000000
Si	0.709763000000	1.101833000000	1.564888000000
Si	0.703401000000	1.106917000000	-1.564033000000
		11h	
C	0.000000000000	0.987220000000	0.000000000000
Ge	-0.001097000000	-1.015249000000	0.000000000000
Ge	-1.837436000000	1.134205000000	0.000000000000
Si	2.457276000000	-1.472123000000	0.000000000000
Si	1.745087000000	0.777129000000	0.000000000000

	12h		
C	0.000000000000	0.704289000000	0.000000000000
Ge	1.566444000000	-0.370200000000	0.000000000000
Ge	-1.456670000000	1.831246000000	0.000000000000
Si	-0.869312000000	-0.916378000000	0.000000000000
Si	0.618400000000	-2.724993000000	0.000000000000
	13h		
C	-0.526497000000	0.871631000000	0.000000000000
Ge	-0.526497000000	-0.193399000000	1.609689000000
Ge	-0.526497000000	-0.193399000000	-1.609689000000
Si	1.223831000000	1.403097000000	0.000000000000
Si	1.408654000000	-0.892545000000	0.000000000000
	14h		
C	1.193259000000	-0.414183000000	0.000000000000
Ge	-0.385513000000	-1.418480000000	0.000000000000
Ge	0.000000000000	1.160351000000	0.000000000000
Si	2.642462000000	0.555974000000	0.000000000000
Si	-2.272686000000	0.211541000000	0.000000000000
	1i		
C	-0.486437000000	0.581107000000	0.000000000000
Ge	-0.157648000000	-1.387706000000	0.000000000000
Si	-0.157648000000	0.524368000000	1.804856000000
Si	-0.157648000000	0.524368000000	-1.804856000000
Si	0.884109000000	1.874118000000	0.000000000000
	2i		
C	1.672427000000	0.226448000000	0.000000000000
Ge	-1.701265000000	-0.739392000000	0.000000000000
Si	0.719073000000	-1.262960000000	0.000000000000
Si	0.000000000000	1.059413000000	0.000000000000
Si	2.452777000000	1.796537000000	0.000000000000
	3i		
C	-0.337094000000	0.531863000000	0.000000000000
Ge	-0.520087000000	-1.428244000000	0.000000000000
Si	0.444413000000	0.402660000000	1.668650000000
Si	0.444413000000	2.231297000000	0.000000000000
Si	0.444413000000	0.402660000000	-1.668650000000
	4i		
C	0.000000000000	0.433133000000	0.000000000000
Ge	-0.655377000000	-1.461284000000	0.000000000000

Si	1.152409000000	1.896350000000	0.000000000000
Si	-1.254065000000	1.757505000000	0.000000000000
Si	1.599661000000	-0.499406000000	0.000000000000
		5i	
C	0.909032000000	0.645921000000	-0.276883000000
Ge	-1.385094000000	-0.424486000000	-0.271403000000
Si	2.487923000000	-0.140965000000	-0.498753000000
Si	-0.379690000000	1.720069000000	0.322084000000
Si	0.668112000000	-0.885674000000	0.915682000000
		6i	
C	0.000000000000	0.761548000000	0.000000000000
Ge	-1.849954000000	0.820022000000	0.000000000000
Si	2.384591000000	-1.703773000000	0.000000000000
Si	0.078684000000	-1.103652000000	0.000000000000
Si	1.765191000000	0.606711000000	0.000000000000
		7i	
C	-0.429631000000	-1.387229000000	0.000000000000
Ge	0.427848000000	1.140169000000	0.000000000000
Si	0.427848000000	-1.013844000000	-1.544149000000
Si	0.427848000000	-1.013844000000	1.544149000000
Si	-1.649508000000	0.016114000000	0.000000000000
		8i	
C	0.635839000000	-1.309055000000	0.000000000000
Ge	-0.516617000000	1.093730000000	0.000000000000
Si	-0.516617000000	-0.934163000000	1.379558000000
Si	1.941570000000	-0.070606000000	0.000000000000
Si	-0.516617000000	-0.934163000000	-1.379558000000
		9i	
C	1.001285000000	-0.868135000000	0.000000000000
Ge	0.000000000000	0.870887000000	0.000000000000
Si	-0.610030000000	-1.570115000000	0.000000000000
Si	-2.362592000000	0.001661000000	0.000000000000
Si	2.543500000000	-0.050088000000	0.000000000000
		10i	
C	0.000000000000	1.192030000000	0.000000000000
Ge	1.223286000000	-0.252203000000	0.000000000000
Si	-1.184105000000	2.475333000000	0.000000000000
Si	-0.327074000000	-2.275641000000	0.000000000000
Si	-1.284903000000	-0.134097000000	0.000000000000

	11i		
C	0.196594000000	0.401371000000	-1.014668000000
Ge	-1.420304000000	0.107230000000	0.000895000000
Si	0.980223000000	-1.251423000000	-0.824564000000
Si	0.761701000000	-0.540679000000	1.350149000000
Si	1.420230000000	1.374990000000	-0.092772000000
	12i		
C	1.056775000000	-0.347642000000	0.000000000000
Ge	0.255418000000	1.408212000000	0.000000000000
Si	0.255418000000	-1.251045000000	1.373680000000
Si	-1.547552000000	-0.567690000000	0.000000000000
Si	0.255418000000	-1.251045000000	-1.373680000000
	13i		
C	1.082647000000	-0.275113000000	0.000000000000
Ge	-0.788178000000	-1.068797000000	0.000000000000
Si	1.082647000000	0.619410000000	1.553201000000
Si	1.082647000000	0.619410000000	-1.553201000000
Si	-0.827737000000	1.322049000000	0.000000000000
	14i		
C	-0.405304000000	1.232418000000	0.000000000000
Ge	1.329324000000	-0.409833000000	0.000000000000
Si	-0.405304000000	0.350365000000	1.561991000000
Si	-2.054146000000	-0.292149000000	0.000000000000
Si	-0.405304000000	0.350365000000	-1.561991000000