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Supporting Information

Transition from exohedral to endohedral structures of $AuGe_n^-$ (n = 2-12) clusters: photoelectron spectroscopy and density functional calculations

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Theoretical results

$AuGe_2^-$

The most stable isomer of $AuGe_2^-$ (2A) is an isosceles triangle structure with C_{2v} symmetry. The calculated VDE of 2A is 2.26 eV, in excellent agreement with the experimental value (2.27 eV). Isomer 2B is a Ge-Au-Ge bend structure with C_{2v} symmetry. It is much higher than isomer 2A in energy by 2.35 eV and its calculated VDE (1.74 eV) is much smaller than the experimental value, indicating that its existence can be ruled out. As we can see from Fig. 3, the simulated DOS spectrum of isomer 2A fits the experimental spectrum of $AuGe_2^-$ cluster very well. Therefore, we suggest that isomer 2A is the most probable one detected in our experiments.

$AuGe_3^-$

The lowest-lying isomer of $AuGe_3^-$ (3A) is a rhombus structure with C_{2v} symmetry. The next low-lying isomer (3B) can be described as the Au atom connecting to one Ge atom of the Ge_3 triangle. Isomer 3C is a tetrahedral structure with the Au atom capping the Ge_3 triangle. Isomer 3D can be regarded as the Au atom adsorbing to the terminal Ge atom of a chain Ge_3 subunit. The calculated VDE of isomer 3A (3.08 eV) is very close to the experimental value (2.97 eV), and the simulated DOS spectrum of 3A is consistent with the experimental spectrum. Thus, we suggest that isomer 3A is the most likely structure observed in our experiments. Isomers 3B, 3C, and 3D can be excluded because they are much less stable than 3A in energy by at least 0.91 eV.

$AuGe_4^-$

As for $AuGe_4^-$, the lowest-lying isomer (4A) can be obtained by the Au atom attaching to the top left of the Ge_4 rhombus. Isomer 4B is a compressed tetragonal pyramid structure with the Au atom located at the bottom. Isomer 4C can be described as the Au atom connecting to the one Ge atom of the Ge_4 tetrahedron. Isomers 4D and 4E both adopt quasi-planar structures with the Au atom located at different positions. The calculated VDE of isomer 4A (3.02 eV) is in good agreement with the experimental measurement (3.17 eV) and its simulated DOS spectrum reproduces the experimental spectrum of $AuGe_4^-$ very well except for the tailed peak centered at 2.80 eV, which could be attributed to the contribution from isomer 4B (VDE: 2.70 eV). Therefore, we suggest isomers 4A and 4B to be coexisted in our experiments, while isomers 4C, 4D, and 4E can be ruled out because they are much less stable than isomer 4A in energy by at least 0.43 eV.

$AuGe_5^-$

With respect to $AuGe_5^-$, isomers 5A, 5C, and 5D all possess a Ge_5 trigonal bipyramid subunit with the Au atom attaching to different positions of the Ge_5 subunit. Isomer 5B can be obtained from isomer 4A by putting an additional Ge atom on the right above of the center of the Ge_4 rhombus. Isomer 5E is a planar butterfly-like structure with the Au atom located at the C_2 symmetric axis. Although the calculated VDEs of isomers 5A, 5B, 5C, and 5D (2.91, 3.21, 3.33, and 3.06 eV) are all in reasonable agreement with the experimental value (3.08 eV), the existence of isomers 5C and 5D can be ruled out because they are much less stable than isomer 5A in energy by at least 0.44 eV. As we can see from Fig. 3, the simulated DOS spectrum of isomer 5A fits the experimental spectrum very well. The DOS spectrum of isomer 5B is similar to the experimental spectrum in some aspects; its energy is slightly higher than 5A by 0.27 eV. Therefore, we suggest isomer 5A to be the most probable structure detected in our experiments, and the existence of isomer 5B cannot be ruled out.

$AuGe_6^-$

The lowest-lying isomer of $AuGe_6^-$ (6A) can be viewed as the Au atom capping the face of the Ge_6 face-capped trigonal bipyramid. Isomer 6B is of C_{4v} symmetry with the Au atom adsorbing to one Ge atom of the Ge_6 tetragonal bipyramid. Isomer 6C can be considered as deriving from isomer 5B by putting an additional Ge atom on the top right of the center of the Ge_4 rhombus. Isomer 6D can be constructed from isomer 5B by adding a Ge atom to the top right of the center of the Ge_4 rhombus. Isomer 6E can be considered as the Au atom adsorbing to one Ge atom of the Ge_6 face-capped trigonal bipyramid. The calculated VDEs of isomers 6A and 6C (2.65 and 2.98 eV) are both in reasonable agreement with the experimental value (2.87 eV), and the combination of their simulated DOS spectra can reproduce the experimental spectrum very well. The energy of isomer 6B is higher than 6A by only 0.01 eV. Although the calculated VDE of isomer 6B (3.34 eV) is much deviated from experimental value, it may make some contributions to the higher EBE regions. Therefore, we suggest that isomers 6A, 6B, and 6C coexist in our experiments, while isomers 6D and 6E can be ruled out because they are much less stable than 6A in energy by at least 0.36 eV.

$AuGe_7^-$

In the structures of $AuGe_7^-$, isomers 7A, 7B, and 7E all have a Ge_7 pentagonal bipyramid unit with the Au atom connecting to different positions of the Ge_7 unit. Isomer 7C can be obtained by the Au atom substituting one Ge atom of the Ge_8 tetragonal prism. Isomer 7D can be viewed as the Au atom absorbing to the edge-capping Ge atom of the Ge_7 capped tetragonal bipyramid. The calculated VDE of 7A (3.42 eV) is slightly higher than the experimental result (3.14 eV), and that

of 7B (3.16 eV) is in excellent agreement with experimental value. As we can see from Fig. 3, the combination of simulated spectra of isomers 7A and 7B can fit the experimental spectrum very well. As a result, we suggest that isomers 7A and 7B coexist in our experiments, and isomer 7B may make major contribution to the lower and higher EBE sides. Besides, isomers 7C, 7D and 7E are much higher than 7A in energy by at least 0.42 eV, indicating their existence can be excluded.

$AuGe_8^-$

In regard to $AuGe_8^-$, the most stable isomer (8A) can be obtained by an additional Ge atom capping the Ge-Ge bond of isomer 7C. The metastable one, 8B can be regarded as the Au atom and one Ge atom face-capping the Ge_7 pentagonal bipyramid, which can also be viewed as an additional Ge atom capping the face of isomer 7B. Isomer 8C can be viewed as the Au atom capping the face of the closely packed Ge_8 tetragonal prism. Isomer 8D can be constructed by an additional Ge atom face-capping the structure of isomer 7C. For isomer 8E, it is a structure with the Au atom edge-capping the Ge_8 tetragonal prism. The calculated VDEs of 8A, 8B, and 8C (3.13, 3.10, and 3.32 eV) are all in reasonable agreement with experimental value (3.37 eV). Besides, isomers 8B and 8C are energetically closed with 8A (higher than 8A in energy by only 0.05 and 0.12 eV, respectively) and their simulated DOS spectra can also duplicate the features of the photoelectron spectrum of $AuGe_8^-$. Even though isomer 8D is slightly higher than 8A in energy by 0.17 eV, the calculated VDE (3.05 eV) is much smaller than experimental value so that its existence can be ruled out. The existence of isomer 8E cannot be excluded because its calculated VDE (3.26 eV) is also in reasonable agreement with the experimental value and its energy is slightly higher than 8A by 0.21 eV. Taking all above into consideration, we suggest that isomers 8A, 8B and 8C are the dominant structures contributed to the photoelectron spectrum of $AuGe_8^-$.

$AuGe_9^-$

As for $AuGe_9^-$ cluster, the lowest-lying isomer (9A) is a multi-rhombus prism with two side-capped Ge atoms, which can be obtained by an additional Ge atom face-capping the bottom of isomer 8A. Isomer 9B can be described as the Au atom connecting to one Ge atom of the Ge_9 tricapped trigonal prism (TTP) structure. Isomer 9C is a bicapped tetragonal antiprism structure with the Au atom substituting one of the two capped Ge atoms. Isomer 9D can be described as the Au atom substituting one Ge atom of the Ge_4 rhombus interacted with the Ge_6 motif and can also be obtained through adding an additional Ge atom to the bottom of isomer 8A. Isomer 9E can be viewed as one Ge_4 rhombus and another Ge_5 pentagonal ring bridged by the Au atom. The calculated VDE of isomer 9A (3.50 eV) is in good agreement with the experimental value (3.60 eV),

and its simulated DOS spectrum fits the experimental spectrum very well. Therefore, we suggest that isomer 9A is the most probable structure detected in our experiments. However, the existence of isomer 9B cannot be ruled out because the calculated VDE of isomer 9B (3.40 eV) is in reasonable agreement with the experimental value and its energy is slightly higher than 9A by 0.25 eV. Isomer 9C can be ruled out because its calculated VDE (3.21 eV) is much deviated from the experimental value, and isomer 9D can be ruled out because its energy is much higher than isomer 9A by at 0.37 eV.

$AuGe_{10}^-$

The lowest-lying isomer of $AuGe_{10}^-$ (10A) is a bicapped tetragonal antiprism with the Au atom adsorbing to one of the two-capped Ge atoms. Isomer 10B can be regarded as deriving from isomer 9B by adding an additional Ge atom to the bottom. Isomer 10C is found to be an endohedrally Au-doped Ge_{10} pentagonal prism with D_{5h} symmetry, which is similar to the most stable structure of $AuGe_{10}^-$ reported in the previous literatures.[28, 30] Our calculations show that isomer 10C is higher than isomer 10A in energy by 0.23 eV. Isomer 10D can be obtained by an additional Ge atom capping the pentagonal face of isomer 9E. Isomer 10E can be described as the Au atom edge-capping the Ge_{10} bicapped tetragonal antiprism. The calculated VDEs of isomers 10A (3.63 eV) and 10B (3.48 eV) are both in good agreement with experimental value (3.55 eV). The simulated DOS spectrum of isomer 10A fits the experimental spectrum very well; that of isomer 10B is also similar to the experimental spectrum and its energy is slightly higher than 10A by 0.20 eV. Thus, we suggest that isomer 10A is most probable structure detected in our experiments and isomer 10B may make some contribution to the broad peak of the photoelectron spectrum of $AuGe_{10}^-$. Isomers 10C, 10D, and 10E can be excluded because the calculated VDE of 10C (3.13 eV) is much deviated from the experimental value and the energies of 10D and 10E are much higher than 10A by at least 0.32 eV.

$AuGe_{11}^-$

As the ground state, isomer 11A is an endohedral structure with the Au atom completely encapsulated into the Ge_{11} cage consisted of one trigonal bipyramid and another one pentagonal pyramid. Isomer 11B can be constructed by the Au atom capping the pentagonal face of the Ge_{11} capped pentagonal antiprism. Isomer 11C can be regarded as the Au atom capping the face of the Ge_{11} face-capped pentagonal prism. Isomer 11D adopts a structure with the Au atom connecting to one Ge atom of the Ge_{11} capped pentagonal prism. Isomer 11E can be considered as a distorted bicapped pentagonal prism with the Au atom substituting a Ge atom of pentagonal prism. The

calculated VDEs of isomers 11A (3.48 eV) and 11B (3.26 eV) are both in good agreement with the experimental value (3.40 eV), and isomer 11B is slightly higher than 11A in energy by 0.13 eV. Moreover, the combined simulated DOS spectra of isomers 11A and 11B fit the experimental spectrum very well. Therefore, we suggest that isomers 11A and 11B coexist in our experiments. Isomers 11C, 11D, and 11E can be ruled out because they are much higher than isomer 11A in energy by at least 0.54 eV.

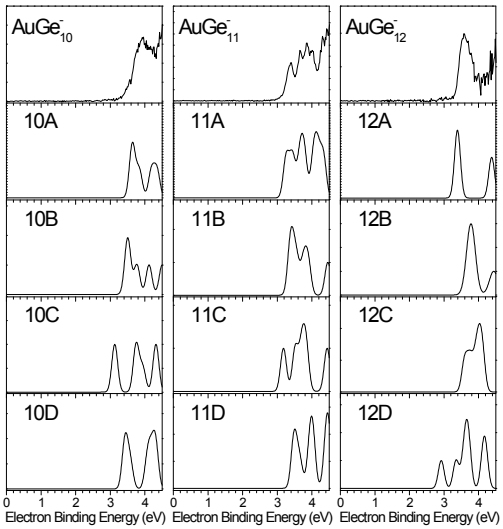
$AuGe_{12}^-$

The lowest-lying isomer of $AuGe_{12}^-$ (12A) is an I_h symmetric icosahedral structure with the Au atom located at the center and twelve Ge atoms situated at its icosahedral vertices. Isomer 12B is a distorted icosahedral structure. Isomer 12C consists of a couple of tetragonal bipyramid, which are separated into two parts by the Au atom. Isomer 12D is a bicapped pentagonal prism structure, in which the Au atom is completely encapsulated into the Ge_{12} cage. The structure of 12D is very similar to the previously results of $AuGe_{12}^-$ calculated at the B3LYP/LanL2DZ level of theory.[29, 30] Isomer 12E can be constructed by the Au atom capping one of hexagonal facets of the Ge_{12} hexagonal prism. The calculated VDE of 12A (3.39 eV) is in reasonable agreement with experimental value (3.60 eV) and that of 12B (3.60 eV) is equivalent to the experimental value, and the energy of 12B is higher than 12A by only 0.07 eV. As we can see from Fig. 3, the combination of simulated DOS spectra of isomers 12A and 12B can reproduce the experimental spectrum very well. Therefore, we suggest that both isomers 12A and 12B contribute to the experimental spectrum of $AuGe_{12}^-$. Isomers 12C, 12D, and 12E are much less stable than isomer 12A in energy by at least 0.31 eV, indicating that their existence can be ruled out.

We have also performed additional calculations about the relative energies of low-lying isomers for $AuGe_{10}^-$, $AuGe_{11}^-$ and $AuGe_{12}^-$ using the PBEPBE, PBE1PBE, B3LYP, and MP2 methods, as well as their corresponding DOS spectra are shown here:

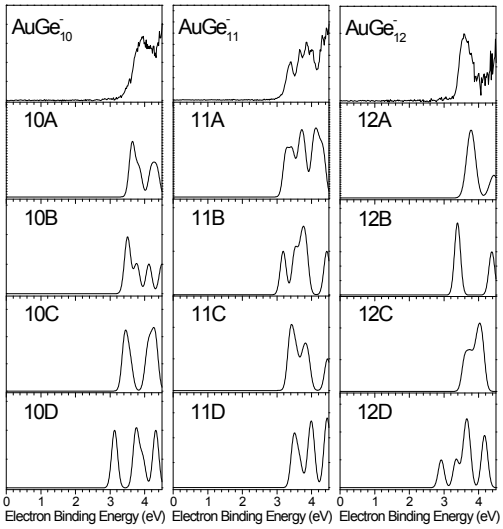
The results of PBEPBE/Def2-TZVPPD//PBEPBE/SDD:

Isomers	Single-Point Energies	Relative Energies
10A	-20903.1872512	0.00 eV
10B	-20903.1785398	0.24 eV
10C	-20903.1507390	0.99 eV
10D	-20903.1681422	0.52 eV
11A	-22979.8824457	0.42 eV
11B	-22979.8978774	0.00 eV
11C	-22979.8868541	0.30 eV
11D	-22979.8834290	0.39 eV
12A	-25056.6330772	0.00 eV
12B	-25056.6282988	0.13 eV
12C	-25056.6306405	0.07 eV
12D	-25056.6171615	0.43 eV



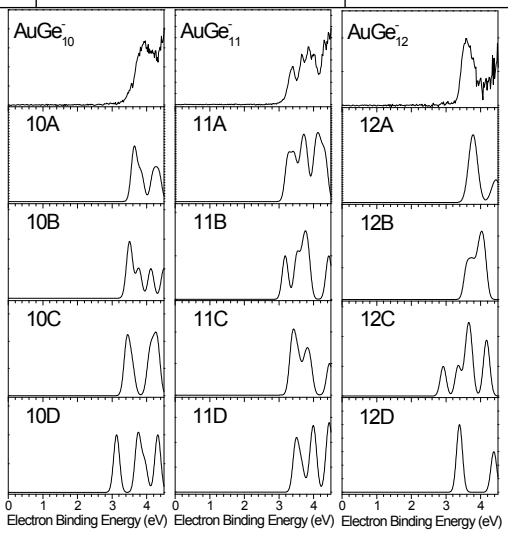
The results of PBE1PBE/Def2-TZVPPD//PBEPBE/SDD:

Isomers	Single-Point Energies	Relative Energies
10A	-20903.6178380	0.00 eV
10B	-20903.6100325	0.21 eV
10C	-20903.5737743	1.20 eV
10D	-20903.5941035	0.65 eV
11A	-22980.3564153	0.46 eV
11B	-22980.3731167	0.00 eV
11C	-22980.3598308	0.36 eV
11D	-22980.3613726	0.32 eV
12A	-25057.1505881	0.20 eV
12B	-25057.1495838	0.22 eV
12C	-25057.1577840	0.00 eV
12D	-25057.1388021	0.52 eV



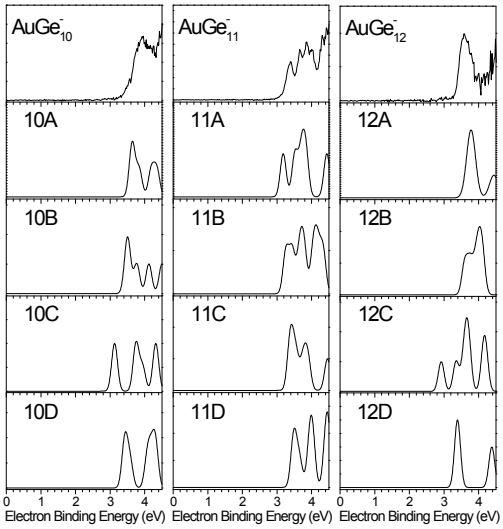
The results of B3LYP/Def2-TZVPPD//PBEPBE/SDD:

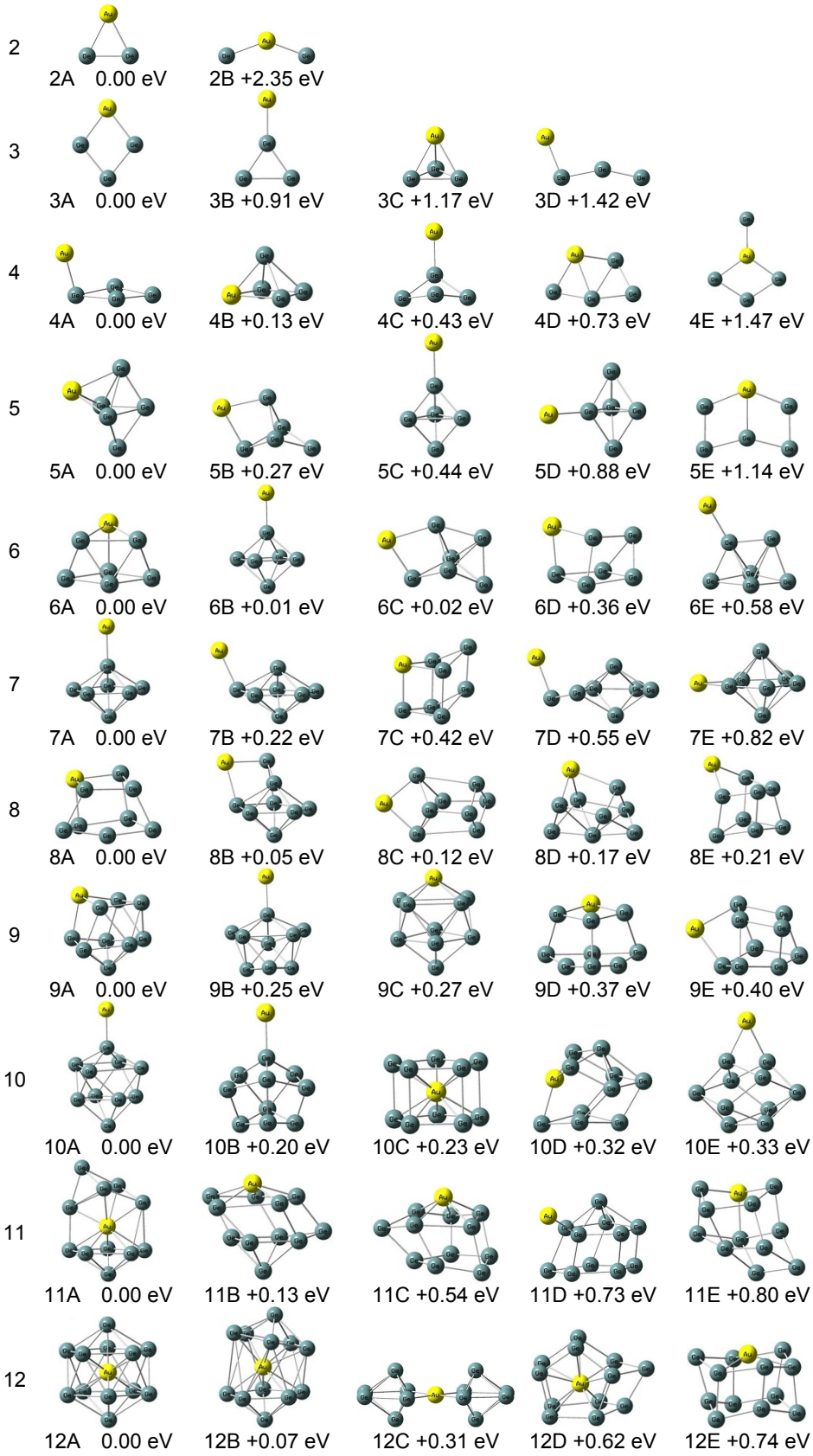
Isomers	Single-Point Energies	Relative Energies
10A	-20906.6753445	0.00 eV
10B	-20906.6662792	0.25 eV
10C	-20906.6253174	1.36 eV
10D	-20906.6473547	0.76 eV
11A	-22983.7052368	0.40 eV
11B	-22983.7200172	0.00 eV
11C	-22983.7174475	0.07 eV
11D	-22983.7176033	0.07 eV
12A	-25060.7826857	0.60 eV
12B	-25060.7909878	0.38 eV
12C	-25060.8048163	0.00 eV
12D	-25060.7840896	0.56 eV



The results of MP2/Def2-TZVPPD//PBEPBE/SDD:

Isomers	Single-Point Energies	Relative Energies
10A	-20888.6948533	0.00 eV
10B	-20888.6924357	0.07 eV
10C	-20888.5954773	2.71 eV
10D	-20888.6402389	1.49 eV
11A	-22964.0045672	1.04 eV
11B	-22964.0194726	0.64 eV
11C	-22964.0188877	0.66 eV
11D	-22964.0429352	0.00 eV
12A	-25039.3562114	1.88 eV
12B	-25039.3856971	1.07 eV
12C	-25039.4250767	0.00 eV
12D	-25039.3733381	1.41 eV





Geometries of the typical low-lying isomers of $AuGe_n^-$ (n = 2-12) clusters optimized at B3LYP/SDD/Au/6-311+G(d)/Ge level of theory. The energies relative to the most stable isomers are calculated at CCSD/aug-cc-pVTZ-PP/Au/cc-pVDZ-PP/Ge level of theory.

Table S1. Cartesian coordinates for the low-lying isomers of $AuGe_n^-$ (n = 2-12) clusters

$AuGe_2^-$

	2A				2B		
	X	Y	Z		X	Y	Z
Ge	1.48051300	1.09909200	0.03876900	Ge	-2.39294400	0.26777300	0.00000000
Ge	0.88666800	-1.23868900	0.02321800	Ge	2.12636200	0.33758400	0.00000000
Au	-0.16473000	1.15527400	-0.00431400	Au	-0.14646100	1.14954100	0.00000000

$AuGe_3^-$

	3A				3B		
	X	Y	Z		X	Y	Z
Ge	-1.33612200	1.79574500	-0.10386600	Ge	-0.01095200	0.78311800	0.02995800
Ge	-2.61621700	-0.25444300	-0.09446200	Ge	-1.37053600	-1.14539300	0.08102600
Ge	-0.34717400	-1.08680300	-0.14390800	Ge	1.30545900	-1.16140200	0.26956600
Au	1.08122500	1.01414500	-0.15534000	Au	0.01854300	3.23782900	-0.16154000
	3C				3D		
	X	Y	Z		X	Y	Z
Ge	0.14045500	6.75234600	2.61405400	Ge	-1.88526600	-0.06066900	-1.32629400
Ge	-2.13287200	6.17664500	2.21008900	Ge	0.29226000	1.37991900	-1.13193300
Ge	2.01995700	8.00615700	2.47988000	Ge	-0.06435900	-0.67450200	0.44857900
Au	-2.27392600	4.02562400	3.44425300	Au	-1.58718900	1.57552600	0.85758900

$AuGe_4^-$

	4A				4B		
	X	Y	Z		X	Y	Z
Ge	1.38203660	1.28773733	-0.19916639	Ge	-0.82572000	1.54609300	-0.00544800
Ge	1.38374243	-1.29060956	-0.18188117	Ge	0.77844200	-0.27420900	0.24229700
Ge	-0.50102313	-0.01054766	-1.37472952	Ge	-1.02473500	-1.90954500	0.08504700
Ge	3.25135724	0.00562760	0.68563773	Au	-3.06992000	-0.06022400	-0.10978100
Au	-2.23437494	0.00315637	0.43347417	Ge	-1.46462500	-0.10122000	1.99054200
	4C				4D		
	X	Y	Z		X	Y	Z
Ge	1.12234882	2.21440308	0.00000000	Ge	-2.32234700	1.04491600	-0.37403500
Ge	-0.43068026	1.65964182	-1.83481576	Ge	-0.75489700	-0.76898000	0.04421100
Ge	-0.71004059	0.05471035	0.00000000	Ge	1.48614500	-1.70410800	-0.25836700
Ge	-0.43068026	1.65964182	1.83481576	Ge	1.74331300	0.69583800	-0.28912700
Au	0.18191565	-2.26380857	0.00000000	Au	-0.26525800	1.79320200	0.87731600

$AuGe_5^-$

	5A				5B		
	X	Y	Z		X	Y	Z
Ge	0.12336500	3.13160100	-0.07764500	Ge	0.17919000	1.97136200	0.11923200
Ge	-1.95497900	1.80926700	-0.79533700	Ge	-2.20080100	-0.17864300	0.24500500
Ge	0.41384700	0.58769700	-0.53333100	Ge	1.23387400	-1.60355800	0.00592800
Ge	-0.30946100	2.87474400	-2.62446300	Ge	-0.01719500	-0.12337600	1.55104200
Ge	-1.52597400	0.29180500	-2.64303000	Ge	-0.20203300	-0.08663500	-1.32799800
Au	1.23347700	0.81976100	-2.97840000	Au	-2.40020000	2.44127000	0.29021500
	5C				5D		
	X	Y	Z		X	Y	Z
Ge	-1.27383600	2.41626600	-0.72024700	Ge	-0.11146900	1.02318400	0.08446700
Ge	-2.98470600	-0.05895800	-0.90202800	Ge	-1.26015300	-1.69730500	-0.05314100
Ge	0.01875100	-0.29291100	-0.99319900	Ge	1.26051400	-1.14142200	-0.32127800
Ge	-1.37229300	0.52950000	0.89526700	Ge	0.22158500	-0.81797400	1.92397100
Ge	-1.45554300	0.85058600	-2.67427800	Ge	-0.30178600	-0.39246300	-2.11657900
Au	-1.31968100	0.30981300	3.34730500	Au	3.48351200	-2.06680300	-0.70246400

$AuGe_6^-$

	6A				6B		
	X	Y	Z		X	Y	Z
Ge	-1.48135900	1.37357000	-0.15194000	Ge	-0.97371600	-0.33861400	1.05943300
Ge	0.60472800	0.60015700	-1.46520100	Ge	-2.86182600	-1.63524500	-0.07554700
Ge	-0.33964200	-1.64024500	-0.35116500	Ge	0.62109700	-1.82264800	-0.30381200
Ge	2.40856600	1.45233600	0.16972500	Ge	-1.12572000	-0.23303000	-1.59557900
Ge	2.20662000	-1.09644400	-0.09234800	Ge	-3.17694900	-1.59044400	-2.61082600
Au	-2.97997600	-0.62866900	-0.46602300	Ge	-0.84179900	-2.65485200	-2.73681800
Ge	0.38098900	0.33275500	1.30458800	Au	-1.28020000	-3.67797800	-0.32577700
	6C				6D		
	X	Y	Z		X	Y	Z
Ge	-1.84979600	-1.41767400	-1.37434200	Ge	0.13177900	0.45575400	-1.27241200
Ge	-1.61592300	1.37617900	-1.47874200	Ge	-1.66133500	-1.21874300	-0.49637800
Ge	0.31167300	-0.16410600	-0.75862600	Ge	0.57232100	-2.00628800	0.73320400
Ge	0.77482100	-1.41304400	1.21095300	Ge	-0.34504100	0.24420700	1.44584700
Ge	-0.54289700	1.37756200	1.11582500	Ge	-2.44346400	1.15228600	0.09713300
Ge	-2.76112200	0.13824300	0.51602500	Ge	-0.15097900	2.49056100	0.26095600
Au	2.59232400	-0.39396500	-1.70784100	Au	2.43846500	-0.87476900	-0.58525400

$AuGe_7^-$

	7A				7B		
	X	Y	Z		X	Y	Z
Ge	-1.23471000	0.90017400	0.62565900	Ge	2.82107000	1.29104000	-0.71513200
Ge	1.37496800	0.83842500	0.68143300	Ge	2.82246100	-1.28955700	-0.71482500
Ge	-2.09801700	-1.56216800	0.53352200	Ge	0.48247800	2.09536400	0.49066000
Ge	2.12436500	-1.66214700	0.62362000	Ge	0.48357200	-2.09644200	0.48980300
Ge	-0.02206200	-3.14578200	0.53216900	Ge	-1.14248100	0.00011900	1.17476900
Ge	-0.00697500	-0.97540500	2.24642100	Ge	1.83034800	-0.00013600	1.35364900
Ge	0.06181200	-0.88235700	-0.88177000	Ge	0.47938700	-0.00011400	-1.13594800
Au	0.11567700	-0.80757800	-3.37311800	Au	-3.15011000	-0.00011100	-0.38196500

	7C				7D		
	X	Y	Z		X	Y	Z
Au	-0.63019700	3.87900700	3.80151600	Au	2.85418700	1.09323500	3.00048000
Ge	1.95828900	4.35114100	1.12063400	Ge	2.34131200	-1.18861600	2.15930000
Ge	-0.79933100	6.25898500	0.89967800	Ge	-0.15852200	-1.03897500	2.34526700
Ge	0.81056600	5.85152600	2.84383900	Ge	1.05347500	-0.42622200	-0.04697100
Ge	-2.30477100	4.30338300	1.80266700	Ge	-1.27736000	0.62359600	0.57028800
Ge	0.56078900	2.31944000	2.03084100	Ge	-0.96862200	-2.08416900	-0.03153300
Ge	-1.71137200	1.95608700	0.68467600	Ge	-3.13417600	-0.81274900	-0.33773900
Ge	-0.36716400	3.81232700	-0.07164400	Ge	-2.60035500	-1.39596700	2.17899700

$AuGe_8^-$

	8A				8B		
	X	Y	Z		X	Y	Z
Au	3.07397000	-1.87081300	2.35854500	Au	-1.07935900	-1.78361000	3.46213100
Ge	0.55018500	-2.14128600	2.29279500	Ge	1.52269400	-1.84821700	3.70031800
Ge	0.16100300	-2.02020100	-0.31828000	Ge	-0.90506300	-2.50904900	0.95315200
Ge	0.31653100	0.24775700	1.61217900	Ge	1.86248200	-2.24912200	1.22276000
Ge	2.46925500	-0.75722300	-0.01312900	Ge	1.82068800	0.30542100	2.40132200
Ge	0.34608700	0.67510300	-1.48935700	Ge	0.26977800	-0.10708100	-0.11839100
Ge	-1.78654100	-0.07946500	-0.13473500	Ge	2.85482200	-0.18429700	0.14071800
Ge	-0.74976000	2.27879100	0.40697500	Ge	-2.13222500	-0.34241700	0.31011100
Ge	1.88356000	1.93635700	0.29800200	Ge	-0.95511600	0.60191500	2.39204800

	8C				8D		
	X	Y	Z		X	Y	Z
Au	2.34462200	-0.56396700	3.54842100	Au	-0.13516000	-4.11763200	2.57141600
Ge	2.51164700	-0.42529400	0.95154100	Ge	1.35078600	-2.15260200	3.26699600
Ge	-0.19588300	-0.67256200	2.97690000	Ge	-1.98871900	-2.36791700	2.80211200
Ge	0.38876500	0.99823500	1.12573500	Ge	-0.59544200	-0.78788400	4.33900400
Ge	0.55472000	-2.07775100	0.97022200	Ge	-2.09076100	-1.35804600	0.16025700
Ge	-0.91842400	-2.65675300	-1.06071400	Ge	-0.30695100	-0.17286200	1.98172000
Ge	0.09494300	-0.42566500	-1.67541000	Ge	2.04023800	-1.09149600	0.73564700
Ge	-2.03771300	-0.61471200	-0.07896900	Ge	0.12340000	-2.63410000	0.03452700
Ge	-1.14087500	1.61813900	-0.85039200	Ge	0.02081900	0.10456900	-0.49764000

$AuGe_9^-$

	9A				9B		
	X	Y	Z		X	Y	Z
Au	0.00632500	-0.00267200	-2.47406000	Au	4.53767400	0.60794500	-1.56375800
Ge	-1.58689300	-1.31198100	-0.92201600	Ge	1.60552700	-1.07513800	0.89411800
Ge	-0.34379400	2.02987700	-0.92088300	Ge	0.08226700	0.52220300	-0.52202200
Ge	1.93451600	-0.71670600	-0.91582600	Ge	2.72364700	0.67545600	2.62817800
Ge	1.98415300	1.64595400	0.31622300	Ge	2.69744300	1.11993700	-0.02737200
Ge	0.42983800	-2.54193000	0.31260000	Ge	1.30761200	3.46622200	-0.04236600
Ge	-2.41706500	0.89917600	0.31007100	Ge	3.33735700	3.09156500	1.57495000
Ge	-1.21376800	-1.00363700	1.79627800	Ge	0.97543300	2.95230900	2.67126200
Ge	-0.26561200	1.55038000	1.79884700	Ge	-0.96009300	2.49917500	0.84481900
Ge	1.47083300	-0.54746200	1.79950100	Ge	-0.10252200	0.35648000	2.24740000

	9C				9D		
	X	Y	Z		X	Y	Z
Au	2.25482600	0.01707000	0.08755500	Au	2.22396200	-0.00010100	1.13137800
Ge	1.07781400	1.94663700	-1.23073000	Ge	0.43521700	-1.80550300	1.35227400
Ge	0.66318400	1.59577500	1.58336200	Ge	-1.52391300	-0.00002700	1.77879400
Ge	-1.24824500	2.16380400	-0.07016900	Ge	0.43533200	1.80539200	1.35241300
Ge	-0.68351100	0.00763300	-1.75774300	Ge	0.82669800	-2.48500800	-1.17621000
Ge	-1.62819800	0.01058200	1.65006400	Ge	1.32867600	0.00005800	-1.42023100
Ge	-2.93337800	0.00335400	-0.65464500	Ge	0.82671600	2.48510100	-1.17603200
Ge	-1.23732500	-2.14640900	-0.06393200	Ge	-1.36217200	1.40856100	-0.96578300
Ge	0.67109800	-1.56380600	1.58753600	Ge	-1.36220100	-1.40847300	-0.96601100
Ge	1.08701200	-1.92109900	-1.22650500	Ge	-3.23835900	0.00001400	-0.17556600

$AuGe_{10}^-$

	10A				10B		
	X	Y	Z		X	Y	Z
Ge	-0.48129800	-0.44920700	-2.19016200	Au	-0.33399300	-1.37894200	-1.81525800
Ge	0.24301800	2.01583600	-1.68683600	Ge	-1.81547400	0.02071200	-0.45684600
Ge	2.00734600	-0.28255900	-1.42644100	Ge	-3.59975100	-0.82922600	1.48852100
Ge	1.81045600	1.59761500	0.38091400	Ge	-0.63691700	2.26590300	0.15016800
Ge	-0.30249100	-2.27756600	-0.42610300	Ge	-1.06854500	-0.03015400	2.04081800
Ge	-2.36189200	0.56392700	-0.78561600	Ge	-1.06050000	2.53319000	2.76907200
Ge	-1.38135200	-0.66356500	1.32053400	Ge	-3.37807300	1.24995900	3.01907400
Ge	-0.91691800	2.06236600	0.70066700	Ge	-4.88318600	1.68211200	0.85902700
Ge	1.41707900	-1.08317800	1.03589000	Ge	-2.95481600	3.50046600	1.16681500
Ge	0.37780900	0.74799400	2.61164800	Ge	-2.98857500	2.42355100	-1.19033500
Au	-0.86625300	-0.99841400	-4.55569000	Ge	-4.31929600	0.00252700	-1.04805200

	10C				10D		
	X	Y	Z		X	Y	Z
Ge	-0.76469800	2.89665300	0.27702500	Au	-1.51331800	-1.20912800	0.98090600
Ge	-2.33519100	0.73578400	0.28486100	Ge	-1.62452600	1.15261000	1.85797700
Ge	-0.76636200	-1.42656900	0.20622100	Ge	-2.15858300	-1.35002300	-1.44888500
Ge	1.77466000	-0.60090600	0.15006300	Ge	-1.58168100	1.22460500	-0.85666100
Ge	1.77576300	2.07118800	0.19394500	Ge	0.54033500	1.95166300	0.81864700
Ge	1.69763600	-0.55450100	-2.63437400	Ge	0.05135400	-0.50485500	-2.34280200
Ge	1.69836300	2.11725300	-2.59013900	Ge	1.12144600	1.78836400	-1.72518900
Ge	-0.84170700	2.94171100	-2.50666300	Ge	2.36346400	-0.12761100	-0.42040800
Ge	-2.41244000	0.78044700	-2.49836100	Ge	0.86677100	-2.20500700	-0.40201900
Ge	-0.84319800	-1.38063500	-2.57740800	Ge	1.19284200	-0.47094800	1.83766800
Au	-0.10130800	0.75781700	-1.16925000	Ge	0.21988400	-2.84335100	2.00054400

$AuGe_{11}^-$

	11A				11B		
	X	Y	Z		X	Y	Z
Au	-0.05092900	0.07976000	0.00060100	Au	-1.31729300	0.41555000	1.43316700
Ge	-2.89409700	-0.55060600	0.00056300	Ge	-2.64508200	-1.26489800	0.02940400
Ge	-1.36724400	-0.94154200	-2.15540400	Ge	-0.30443700	-2.35348900	-0.55149800
Ge	-1.36585600	-0.94647200	2.15494200	Ge	0.23074500	-1.68365700	2.01882400
Ge	-0.94933100	-2.62537500	-0.00226100	Ge	2.15856100	-1.37677200	0.32846000
Ge	-1.98740200	1.60477600	1.30518600	Ge	1.23553600	-1.07798700	-2.34356700
Ge	-1.98825500	1.60801100	-1.29938300	Ge	1.22967700	0.98338500	1.57547700
Ge	1.58538100	-1.97434500	-0.00173000	Ge	1.47575900	1.37007800	-1.22111000
Ge	2.22861500	0.87150000	-1.35593700	Ge	3.40967200	0.94382900	0.37782200
Ge	2.22986700	0.87119300	1.35490000	Ge	-1.01025000	0.05516200	-1.86875400
Ge	0.87790400	2.63050700	0.00038000	Ge	-0.54968300	2.49845000	-0.15812400
Ge	3.78622100	-0.65280100	-0.00131300	Ge	-2.91042500	1.30705300	-0.72528400

	11C				11D		
	X	Y	Z		X	Y	Z
Au	-0.20310800	1.00292200	1.98712300	Au	-3.84294900	-0.10002200	0.05165000
Ge	-3.52020000	1.96481600	0.44020300	Ge	-1.42098200	-0.31471300	-0.39505600
Ge	-2.13420100	-0.29929400	0.65494100	Ge	-0.27717800	-2.44425000	-1.07595100
Ge	-1.86248300	1.64090700	-1.40833000	Ge	-0.13497200	1.25472900	1.45989400
Ge	-1.16910400	-0.84611000	-1.59724000	Ge	-0.18492300	-1.38696300	1.80334800
Ge	0.94341200	-0.84469700	0.39816500	Ge	2.13845600	-0.08740000	2.01815600
Ge	1.30249100	-1.21303800	-2.11158000	Ge	1.95993700	-2.26719100	0.38851100
Ge	2.20174800	1.06340100	-1.39408300	Ge	2.12293400	1.58031600	-0.04398300
Ge	0.41169200	2.93019900	-1.26863500	Ge	3.55735800	-0.43284200	-0.64457300
Ge	2.02133300	2.05002000	0.90606300	Ge	1.37698400	-0.63117100	-2.01280300
Ge	0.81201900	4.41363100	0.70930000	Ge	0.50793500	3.46932200	-0.02326600
Ge	-1.34615500	3.11336500	1.14142300	Ge	-0.15826700	1.50709300	-1.60178800

$AuGe_{12}^-$

	12A				12B		
	X	Y	Z		X	Y	Z
Ge	-1.94651100	-0.03538200	-1.96355900	Ge	1.36045100	1.88689400	-1.34778800
Ge	-1.60479000	2.24358700	-0.19115600	Ge	1.68855200	-0.67185400	-2.16683700
Ge	1.21456300	2.43442400	0.49359500	Ge	1.89635200	-2.23479700	-0.02105500
Ge	2.61523500	0.27337300	-0.85548700	Ge	1.69268900	-0.71207400	2.15358000
Ge	0.66171000	-1.25302100	-2.37425000	Ge	-1.32587900	2.32686200	0.02788000
Ge	0.42060600	1.63824500	-2.18730100	Ge	-1.50268300	0.73714000	-2.17115600
Ge	-1.21456200	-2.43442500	-0.49359600	Ge	-1.83408500	-1.83464600	1.30232700
Ge	1.60479000	-2.24358700	0.19115700	Ge	1.36309200	1.86092200	1.38253700
Ge	1.94651100	0.03538200	1.96355900	Ge	-1.50894800	0.68457900	2.18738900
Ge	-0.66171100	1.25302100	2.37424900	Ge	-1.83024100	-1.80312900	-1.34660800
Ge	-2.61523500	-0.27337300	0.85548600	Ge	3.09594000	0.18389300	0.00055800
Ge	-0.42060600	-1.63824500	2.18730100	Ge	-3.09645000	0.17250700	0.00007300
Au	0.00000000	0.00000000	0.00000000	Au	0.00049100	-0.24153800	-0.00036500

	12C				12D		
	X	Y	Z		X	Y	Z
Ge	-1.66882600	0.22766800	-3.87046900	Ge	-2.52933700	0.82579900	1.26677900
Ge	-0.57940500	-0.95770400	-1.73693800	Ge	-2.02932300	-1.73766500	1.28982000
Ge	0.85763200	0.21077100	-3.65707500	Ge	0.69068500	-1.73003000	2.08463800
Ge	-2.77553500	0.59055100	-1.42243100	Ge	1.67425600	0.67424300	1.89874500
Ge	-0.53560800	1.92906400	-2.15616400	Ge	-0.37855300	2.25326200	1.40407300
Ge	1.54248500	0.58801800	-1.06106900	Ge	1.65589900	0.78563300	-1.86033200
Ge	-3.05429000	1.15446200	1.91667200	Ge	-0.35723000	2.34440600	-1.23469000
Ge	-0.89505200	2.62850000	2.60557800	Ge	-2.49709100	0.91296700	-1.24645400
Ge	1.25976200	1.01181700	2.29853400	Ge	-2.01984900	-1.64428400	-1.40053200
Ge	0.15426000	1.42096200	4.73980700	Ge	0.67516900	-1.60934700	-2.16984200
Ge	-2.37086800	1.48518300	4.51943100	Au	-0.27154500	-0.09479500	0.00437900
Ge	-1.01770900	-0.25672100	3.01948000	Ge	3.55971800	0.65354800	-0.00295300
Au	-0.75682500	0.83603800	0.43299100	Ge	2.22603300	-1.49450700	-0.04006400