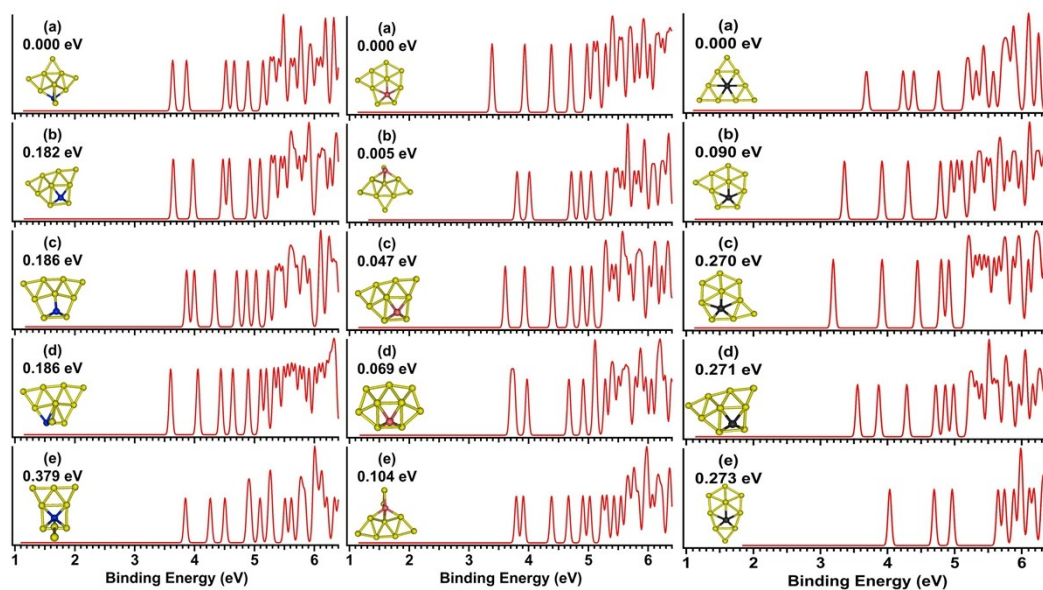
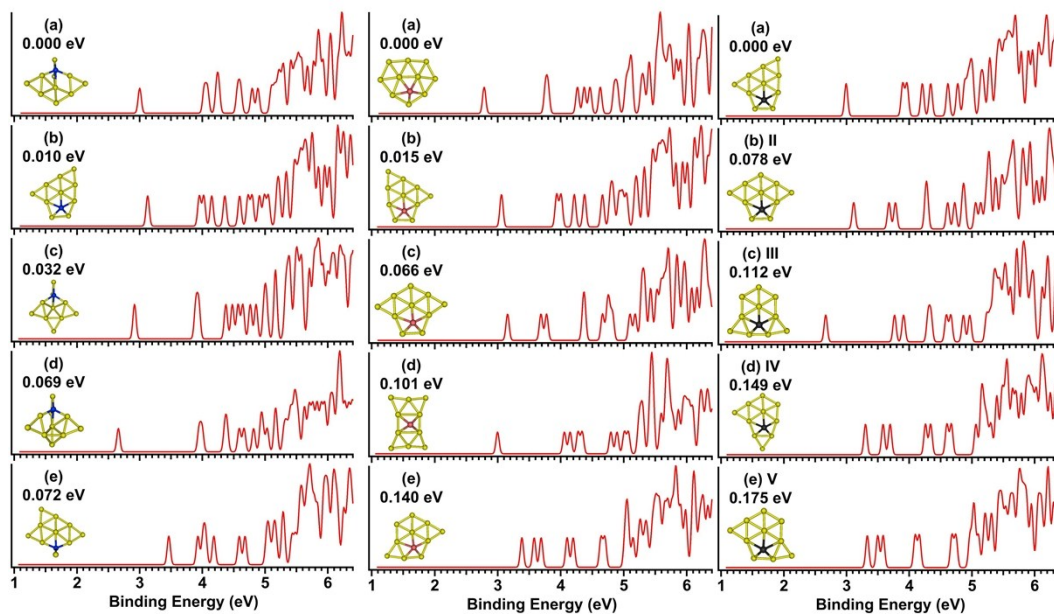


### Supporting information:

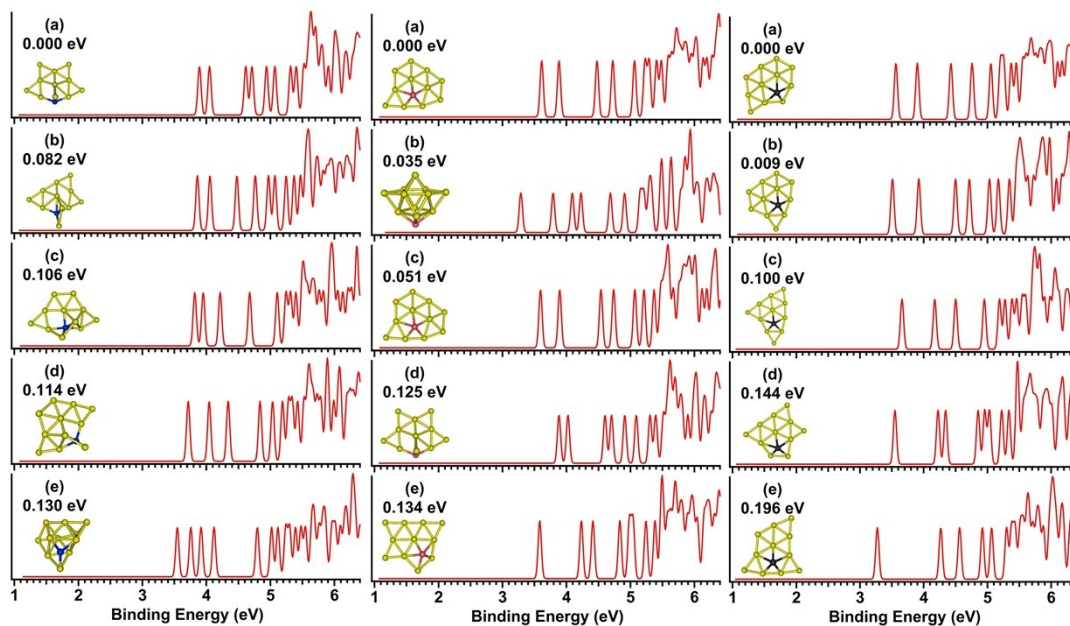
**Fig. S1.** The simulated PES spectra of the top-five lowest-lying isomers of  $\text{Au}_9\text{Si}^-$  (left, a-e),  $\text{Au}_9\text{Ge}^-$  (middle, a-e), and  $\text{Au}_9\text{Sn}^-$  (right, a-e). For each species, the isomers are numbered from the top to bottom (i.e. a-e) as isomer 1 to 5 in accordance with those in Table 1. The relative energies of five low-lying isomers were obtained by PBE0/CRENBL level of theory (NWChem). The insets show the corresponding structures. The dopant atoms are shown in color (Si in blue, Ge in red, and Sn in black).



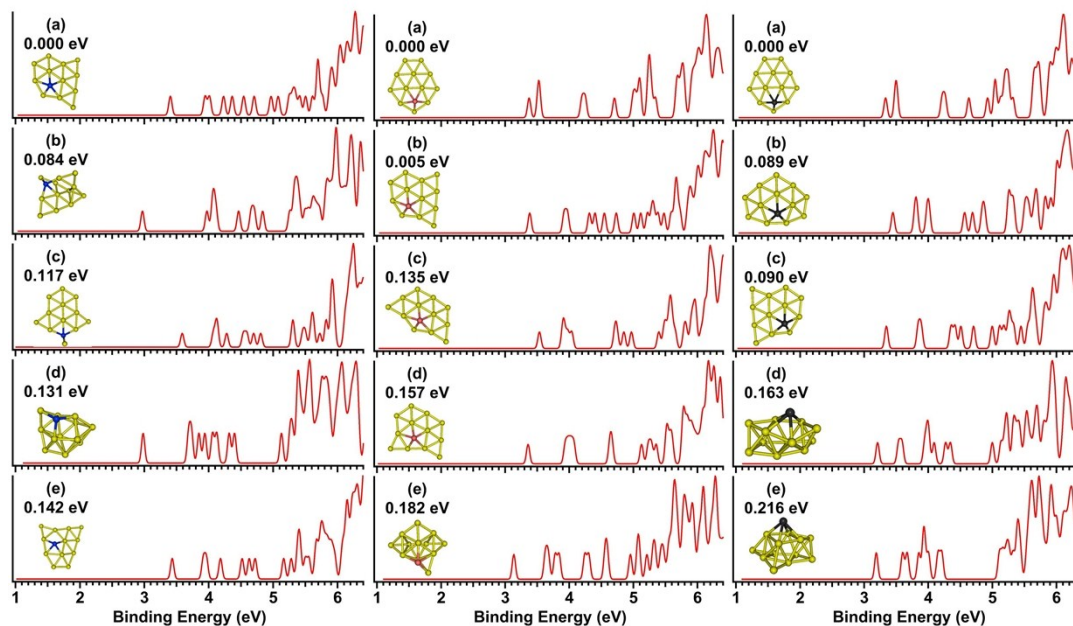
**Fig. S2.** The simulated PES spectra of the top-five lowest-lying isomers of  $\text{Au}_{10}\text{Si}^-$  (left, a-e),  $\text{Au}_{10}\text{Ge}^-$  (middle, a-e), and  $\text{Au}_{10}\text{Sn}^-$  (right, a-e). For each species, the isomers are numbered from the top to bottom (i.e. a-e) as isomer 1 to 5 in accordance with those in Table 2. The relative energies of five low-lying isomers were obtained by PBE0/CRENBL level of theory (NWChem). The insets show the corresponding structures. The dopant atoms are shown in color (Si in blue, Ge in red, and Sn in black).



**Fig. S3.** The simulated PES spectra of the top-five lowest-lying isomers of  $\text{Au}_{11}\text{Si}^-$  (left, a-e),  $\text{Au}_{11}\text{Ge}^-$  (middle, a-e), and  $\text{Au}_{11}\text{Sn}^-$  (right, a-e). For each species, the isomers are numbered from the top to bottom (i.e. a-e) as isomer 1 to 5 in accordance with those in Table 3. The relative energies of five low-lying isomers were obtained by PBE0/CRENBL level of theory (NWChem). The insets show the corresponding structures. The dopant atoms are shown in color (Si in blue, Ge in red, and Sn in black).



**Fig. S4.** The simulated PES spectra of the top-five lowest-lying isomers of  $\text{Au}_{12}\text{Si}^-$  (left, a-e),  $\text{Au}_{12}\text{Ge}^-$  (middle, a-e), and  $\text{Au}_{12}\text{Sn}^-$  (right, a-e). For each species, the isomers are numbered from the top to bottom (i.e. a-e) as isomer 1 to 5 in accordance with those in Table 4. The relative energies of five low-lying isomers were obtained by PBE0/CRENBL level of theory (NWChem). The insets show the corresponding structures. The dopant atoms are shown in color (Si in blue, Ge in red, and Sn in black).



The Cartesian coordinates of the top-five lowest-lying isomers of  $\text{Au}_9\text{Si}^-$

Isomer (a)

Au	1.1482026583	-2.0134283776	-0.9294564826
Au	-1.2748710188	-1.3680331806	0.1876122760
Au	-0.8794368281	-3.8090996430	-0.8405471742
Au	3.7765672237	-0.0405355599	1.1398453946
Au	-1.2470829823	1.3936597041	0.1974063616
Au	-3.4070641038	0.0315295847	0.9911960373
Au	-0.8019689300	3.8336982229	-0.8123907867
Au	1.1885194553	1.9974894182	-0.9155394620
Au	0.9976035016	-0.0138655976	1.2073394880
Si	2.5020526403	-0.0213368581	-0.9234884800

Isomer (b)

Au	-3.1141324756	1.3128464208	0.7023078208
Au	2.0010923675	1.3990976474	0.0726142309
Au	-2.6306256451	-1.3478586614	-0.0816308228
Au	-0.7413417866	2.4079351042	-0.3122644371
Au	1.3685575219	3.9972450893	0.1988042796

Au	-0.0368285934	-0.1894340657	-0.8968016638
Au	2.2499710900	-1.2336473365	0.2082220171
Au	1.9690772137	-3.9294445697	0.5348875120
Au	-0.3118220665	-2.7197517372	0.0112866907
Si	-2.3016966198	0.6587203240	-1.5209195581

Isomer (c)

Au	0.4932656625	-2.5515247923	0.0522919234
Au	0.1683898969	-0.0021022506	-1.0101690714
Au	-1.6672769289	3.9843040008	0.3264513428
Au	-1.7493121713	-3.9499856984	0.3225797321
Au	-2.0612705127	1.3337532671	-0.0124632834
Au	-2.0886672216	-1.2911753962	-0.0115111296
Au	2.9323353319	-1.4792800349	0.3161265453
Au	0.5460289210	2.5410804901	0.0502844584
Au	2.9634156584	1.4211155950	0.3140423105
Si	2.5121252739	-0.0258645532	-1.5825209378

Isomer (d)

Au	0.5127284891	-2.5309633304	-0.6573832225
Au	2.5461488480	1.1379259548	-1.2580012295
Au	-1.7642865562	3.9241852116	0.0449376618
Au	-1.7536342167	-3.9440701637	-0.4734881218
Au	2.9929824262	-0.6913968681	1.6476910836
Au	0.4798135284	-0.0106486596	0.6410330514
Au	-1.9235026891	-1.3723540097	0.2784758618
Au	0.3828904265	2.4974874984	-0.5417617930
Au	-1.9868053104	1.2541490579	0.4675267931
Si	2.5258226738	-1.1892142049	-0.6744856715

Isomer (e)

Au	-0.4630390341	-0.9724231029	2.6253815515
Au	-1.3517285907	0.8247518938	0.6675973185
Au	2.1810150549	-0.9349248087	1.5614203736
Au	2.1547163188	3.2216824284	-1.5835174162
Au	-0.5988734019	-5.6267579632	-1.6979086173
Au	-0.3158756945	3.0155606847	-0.6809036611
Au	-0.2117539232	-3.2926885318	-0.6514809550
Au	-2.7289335461	3.1486500704	0.3779273523
Au	1.4203999359	0.8653589610	-0.4473274154
Si	0.1146723103	-1.1310732028	0.2376513086

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>9</sub>Ge<sup>-</sup>

Isomer (a)

Au	3.0849737467-1.4173375710	0.1528409894
Au	0.6833751868-2.6756826367	0.0581479196
Au	3.2844330433 1.3907652478	0.0238030083
Au	0.8944226746 0.0616736902	-0.2815889822
Au	-1.5857586467 -1.0861763206	-0.1471959693
Au	-1.7856423550 -3.7543082359	0.1778628379
Au	0.9115155053 2.7505554848	0.0151930721
Au	-1.7152683912 3.2248901875	0.3561172566
Au	-3.3390204670 0.9604373707	0.0959716785
Ge	-1.1712553166 1.3236174966	-1.2746960107

#### Isomer (b)

Au	1.2764084284-1.4062877677	-0.1833428111
Au	1.3307613878 1.3537801570	-0.1839750697
Au	-0.9577058120 0.0187468098	-1.1841188502
Au	-1.0856967026 2.0579074993	0.8948117022
Au	-3.7180305063 0.0741458369	-1.2036038504
Au	0.8206541015-3.8569404468	0.7923520582
Au	-1.1667842926 -2.0145534139	0.8936093002
Au	0.9732060652 3.8202480098	0.7926872854
Au	3.4453089209-0.0687793437	-0.9896365114
Ge	-2.5074909393 0.0491221093	0.9691556720

#### Isomer (c)

Au	2.8450380763-0.6142605358	-0.0866030292
Au	-1.8781331333 -1.7805351534	-0.1244303753
Au	-0.9209560816 -4.3291511005	-0.3566897806
Au	2.6265149975 2.0677726133	-0.8407176984
Au	-2.3105887965 0.8320223804	-0.0588860669
Au	0.0871554171 2.5240395738	0.2532331597
Au	0.0975671655-0.1504626056	0.8622874594
Au	0.9910910058-2.5638092144	0.0516465010
Au	-2.3711224017 3.5011823460	-0.2457090341
Ge	2.1218591303 1.2628494093	1.4816715333

#### Isomer (d)

Au	-2.0692501327 2.6794621013	0.3717281355
Au	0.6206112515 3.5038426580	0.4085615341
Au	0.6062638710-3.5014740096	0.3893914937
Au	2.3879846011 1.3580929186	0.5161834935
Au	-0.1013741105 -1.3112406228	-0.9526580816
Au	-2.4113204968 0.0070358572	0.0083442220
Au	-2.0823522113 -2.6713461857	0.3545813065
Au	2.3852608867-1.3680910245	0.5129913143

Au	-0.0907884648	1.3194299690	-0.9402569434
Ge	2.0472040096	-0.0030061365	-1.6374786589
Isomer (e)			
Au	2.2345289719	3.5284038789	0.5239147413
Au	0.0960886969	-0.0255222522	-1.3595798193
Au	1.0716297093	-4.0332124848	0.5408792812
Au	-0.6475708740	-1.9974047199	0.7565596999
Au	2.4266104394	0.9698260774	-0.3183714185
Au	2.0298386739	-1.6553435837	-0.3093935541
Au	-0.0181649125	2.1056135182	0.7444474565
Au	-2.5093635550	0.3879204420	-1.5816270041
Au	-4.0545744745	0.6235066662	0.7426309926
Ge	-1.6001631940	0.2489675346	0.8108733268

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>9</sub>Sn<sup>-</sup>

Isomer (a)

Au	0.1145809636	2.6679055040	0.0559762516
Au	2.4284435564	1.1001298820	0.0132149127
Au	-2.4171821570	-1.2425515838	0.2251585965
Au	-0.2701034935	-2.6966696459	0.1949496572
Au	-2.2210820612	1.5442165390	0.1469996792
Au	2.2452335991	-1.4856423287	0.0765217428
Au	-4.6077594253	0.3089272553	0.0857711549
Au	2.5510067698	3.7771205435	-0.1891277314
Au	1.9763842060	-4.1585275932	-0.0096717886
Sn	-0.0586154414	-0.0467863424	-1.0593993822

Isomer (b)

Au	1.6890187220	3.2648765306	-0.4429094376
Au	-0.9355946050	2.7138024533	-0.0934423229
Au	-3.3066363480	1.3526891260	-0.1182435131
Au	-0.7232847799	-2.7140172417	-0.0173136285
Au	1.7263189643	-3.8260548365	-0.2050826552
Au	1.5655173063	-1.1484780922	0.1179082787
Au	-0.9274663048	0.0235656448	0.3139340558
Au	3.2693420227	0.9247456371	-0.3086227507
Au	-3.1206326813	-1.4526111136	-0.1721925897
Sn	1.2302042290	1.3678052662	1.4947989891

Isomer (c)

Au	-3.0216289101	0.8751888433	0.0806574441
Au	-1.4148776172	-1.3192427812	-0.2010110990
Au	2.6392358564	1.2862399048	-0.0237597536
Au	0.9254817326	3.4465434768	0.0510921279

Au	-1.7901684062	3.2941541830	0.3446913081
Au	0.7930831198	-2.8912580173	0.2402421140
Au	-1.7441885085	-3.9460298062	0.1315914623
Au	-0.2671274577	1.0705434855	-0.2750014895
Au	2.9950357677	-1.3422408684	0.6087073848
Sn	1.4067742834	-0.7485798047	-1.5179406387

Isomer (d)

Au	0.1459093773	2.4957290716	0.2529217859
Au	0.7851371251	-2.6480573765	0.0086459355
Au	2.6382143517	1.9108028561	-0.9223613613
Au	-2.2718788717	3.5826996547	-0.2513598392
Au	-2.3246883491	0.9119778366	-0.0985400045
Au	-2.0198545400	-1.7154937481	-0.1846076386
Au	2.7312933616	-0.8112046372	-0.2633464821
Au	-1.2152570809	-4.3133917616	-0.4126818239
Au	0.0231485701	-0.1896540611	0.8604061060
Sn	2.2950185654	1.1174711174	1.6318184324

Isomer (e)

Au	-2.3118392262	2.6460278846	0.1938449312
Au	-0.0013486552	1.6364183619	-0.6822929047
Au	0.0035545238	-4.9017062190	0.6506342554
Au	2.1449561660	-0.0963240182	-0.0940243908
Au	-2.1452711331	-0.0985642604	-0.0899088367
Au	2.3079763899	2.6489500146	0.1923283972
Au	-1.4234173336	-2.6589441152	0.1002733379
Au	-0.0027936815	4.0878396196	0.6741061690
Au	1.4280719931	-2.6579514160	0.0969791028
Sn	-0.0012971170	-0.9701576102	-1.6700384390

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>10</sub>Si<sup>-</sup>

Isomer (a)

Au	-2.1000685036	-0.0052837335	-1.8253345833
Au	0.5827338796	4.4258965098	0.8839852182
Au	-0.8316051239	2.1551786688	0.7763209868
Au	0.4073600758	-0.0058993168	-0.8920355708
Au	1.8451033612	2.3164562559	-0.1767669887
Au	-4.2064042235	0.0065731796	0.0166178386
Au	3.1024921925	-0.0078753945	-0.6846754905
Au	1.8421010169	-2.3226938241	-0.1431832211
Au	-0.8366829778	-2.1364491492	0.8051753097
Au	0.5643199930	-4.4143060956	0.9346266572
Si	-1.8708291227	0.0099745353	0.6605965112



Isomer (b)

Au	-2.7700941156	-0.4003591081	0.0486016082
Au	-3.3227646855	2.2344639730	-0.2932015828
Au	-1.0510386205	3.8968032473	-0.1151599749
Au	0.1586405210	-4.8849741441	-0.1332459823
Au	3.6931197114	2.3444399854	-0.1535159137
Au	1.0371817267	2.2029581690	0.1133989855
Au	-1.4239133878	-2.7208620948	0.0019616061
Au	2.6267114680	-0.1254365710	-0.0309978551
Au	-0.0791761160	-0.3235272118	0.2975981217
Au	1.4625278663	-2.5256932480	-0.0627093896
Si	-1.3634790494	1.7380037684	1.1663197681

Isomer (c)

Au	3.7786022311	-1.3417901943	0.6923148596
Au	0.2606242304	4.5846831230	0.5747055519
Au	-0.0110520783	0.2881434298	-1.3547431836
Au	2.0568545332	0.7206318471	0.6946629178
Au	-1.9275426405	0.9327991738	0.7832661437
Au	-3.8573380394	-0.9343368949	0.8641974623
Au	1.2805073070	-1.8620883102	-0.1106414764
Au	-0.2242379096	-4.0398483252	-0.5734853598
Au	0.1243675565	2.9438561196	-1.7303288930
Au	-1.4673149550	-1.7160412444	-0.0492343589
Si	0.1326629658	2.1527337815	0.6265458768

Isomer (d)

Au	2.5106250452	-3.5532443502	0.7924012930
Au	1.6669241255	-2.2584061252	-1.5365766654
Au	0.1406318667	-0.1117031646	-1.3519493580
Au	-3.8701095373	-0.9761313775	0.9766832914
Au	0.0116008341	2.3791204183	-0.0630561281
Au	1.9684368888	0.6403511956	1.0108471133
Au	-1.2898116083	1.9473799372	-2.4860668073
Au	2.2068017675	3.3162945417	1.1410406961
Au	-1.2663750906	-1.6487293225	0.9163154755
Au	-2.2110309006	0.8082088522	-0.1206595236
Si	1.1088855314	-1.5690473292	0.7939351862

Isomer (e)

Au	-1.6558354726	-3.9345589130	0.8711645950
Au	-2.1164445453	-1.3235286221	0.5569371478
Au	-3.8388676104	1.4194022620	-1.6067283965

Au	2.9563899928	-3.1510564665	-0.4935044197
Au	1.2321996011	4.5511239020	0.7521009750
Au	-0.8339974861	2.8545320047	0.5684325191
Au	0.4345345149	-2.4900649334	0.0461764703
Au	1.9166768256	2.0697155864	-0.0075051509
Au	-0.0749408396	0.2738408337	-0.3654078505
Au	2.5103849001	-0.5101914803	-0.3884970841
Si	-2.4216702311	1.0601877527	0.2479329032

The Cartesian coordinates of the top-five lowest-lying isomers of Au10Ge<sup>-</sup>

Isomer (a)

Au	-2.5662327108	2.7481740803	-0.1535476785
Au	-2.5950272225	-2.7116095844	-0.1732209722
Au	-0.3342268535	-1.3304271045	0.3387557345
Au	2.1753075322	-2.3250171957	-0.0120980801
Au	-0.0088407500	3.9771420862	-0.1839361073
Au	-0.3205973617	1.3348387552	0.3411061561
Au	2.2012046880	2.2941488578	-0.0204510014
Au	3.5932819066	-0.0237042710	-0.4046371737
Au	-2.7371512804	0.0178814467	0.0073545502
Au	-0.0565958121	-3.9780398669	-0.1829495392
Ge	1.7537677080	-0.0099353863	1.3409167429

Isomer (b)

Au	0.0551557267	0.3326799816	-0.2863637099
Au	2.7379008196	-0.0150079825	-0.1526511135
Au	-1.1368236557	2.7506407233	-0.0233421834
Au	1.7553358629	2.4913198430	-0.2012806376
Au	2.9813261369	-2.6747844519	0.3326339764
Au	-1.3863373215	-2.0073589417	0.0245134246
Au	0.4663092059	-3.9524320087	0.3311091066
Au	-2.6338081305	0.5400591827	0.0914741567
Au	-4.0285307466	-1.7444206492	0.3567817913
Au	0.5261857004	4.8751098951	-0.1037298097
Ge	1.0421636075	-1.9398739551	-1.1698894756

Isomer (c)

Au	-0.3916577772	2.5221387806	-0.1043910655
Au	-1.2109583641	-2.1203675817	-0.1989758220
Au	2.3735041702	2.0497999947	0.0815991022
Au	3.2431090622	-0.5188255635	0.1209162258
Au	1.5469877496	-2.6309627939	-0.0116105946
Au	-0.2343132446	-4.6288914249	0.0183827705

Au	0.5878485755-0.0429377581	-0.2297087146
Au	-3.0028647607 1.9860444200	0.2917230258
Au	-3.4844588331 -0.7397571009	0.2346940077
Au	1.3838723037 4.5342967530	0.1999809996
Ge	-1.7313317567 0.3883677040	-1.2860123177

Isomer (d)

Au	-2.5264426080 -3.8685340081	0.3004139336
Au	2.6967069087-3.7491835323	0.3102798135
Au	-2.6987116154 3.7511759780	0.3017482508
Au	-1.6451015014 1.2992550632	-0.2643618591
Au	-1.5872782406 -1.3692431503	-0.2623440100
Au	2.5245915540 3.8696557487	0.3089678941
Au	1.5859393062 1.3718698287	-0.2585727612
Au	-0.0809269355 3.5509395439	0.1705753892
Au	0.0793394210-3.5471906669	0.1683363473
Au	1.6480091295-1.2968355214	-0.2593695512
Ge	0.0029606212-0.0009487903	-1.7513617803

Isomer (e)

Au	3.1998077114-0.8795899991	0.0725235625
Au	-0.0581877056 -4.8411047554	0.2209079722
Au	0.9193971408-2.3377261433	-0.0935187500
Au	-3.1180097425 -0.4917858622	0.3698713015
Au	-1.6701542828 4.4028037139	0.1688550888
Au	3.0681427171 1.9146151286	0.1587679943
Au	0.7183963803 3.1927663313	0.0600648832
Au	-1.6071005360 1.7249806744	-0.2454590012
Au	0.8349989050 0.4019679069	-0.2310124323
Au	-1.8141399577 -2.8331466283	-0.0242929845
Ge	-1.2145194910 -0.6617454954	-1.3180526302

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>10</sub>Sn<sup>-</sup>

Isomer (a)

Au	0.2446732923 4.9683807312	-0.0319739428
Au	1.1193076401-2.1454086730	0.0641783947
Au	-2.6958824144 0.4756333154	-0.0749698972
Au	-3.4139690579 -2.1152863152	0.3584878633
Au	-1.0564153661 -3.7092511513	0.5007599314
Au	2.7146724279 0.2020031361	0.0822457862
Au	0.0185454692 0.3979480350	-0.2482231833
Au	-1.3244537569 2.7936137306	-0.1275528492
Au	1.5722968246 2.6172769905	0.0029996233

Au 3.7869870506-2.2497690566 0.3415535286  
Sn -1.3477514495 -1.7725492554 -1.4234702902

Isomer (b)

Au -0.8255787944 -4.6274242722 -0.1916773016  
Au -2.1131985040 -2.2860963588 -0.0422836867  
Au -3.3264573248 0.1360565194 -0.1249860127  
Au -0.6289849589 0.0288622952 0.2855455219  
Au 0.6903072184-2.4008881377 0.1059609153  
Au 3.2061898983-1.5262113618 -0.3819724367  
Au 3.3220937640 1.2658172286 -0.3925912670  
Au 0.8842187668 2.3416477957 0.0832023184  
Au -1.9205314478 2.4534139570 -0.0574743900  
Au -0.4492122472 4.6809122021 -0.2327406831  
Sn 1.8522597346 -0.0650853158 1.5219844452

Isomer (c)

Au -3.8455356487 -1.1272332467 -0.4041092642  
Au 0.9572123134 4.4453327032 -0.3002069290  
Au 2.9303672278-0.5264741950 -0.2925798080  
Au -0.5528928092 2.2738502665 0.2067869853  
Au -1.2362690374 -0.3610892550 0.2437450806  
Au 0.7616836208-2.2096076690 0.2121682839  
Au 3.2050224758-3.2259492099 -0.2851975763  
Au -1.8731906005 -2.9739405019 -0.0519011549  
Au -3.1831738119 1.4931573428 -0.0575493053  
Au 2.1810949983 2.0244737718 -0.2980860114  
Sn 1.0782296198 0.3193903742 1.6378430821

Isomer (d)

Au -0.6834240917 -4.9615256185 -0.4793227948  
Au -1.3602218491 2.9555877171 -0.1534669075  
Au 1.2764334945-3.0929654280 -0.1533731569  
Au -3.8525656264 2.0330476697 -0.0376523057  
Au -1.5022747601 -2.4245867160 -0.1181173431  
Au 0.7206276671 1.2206609275 0.2705666936  
Au 3.3374788885 1.8379991659 -0.0668264307  
Au 2.5863753030-0.7904356467 0.0082110686  
Au -1.8722300056 0.1889510098 0.1614175093  
Au 1.1902669029 3.7742713667 -0.4532033296  
Sn 0.2520854676 -1.1778038999 1.6317235261

Isomer (e)

Au -3.2648581692 0.8144431353 -0.0223365747  
Au 3.1580193445 0.5208507428 -0.3111309057

Au	-0.8817715079	-0.4453555330	0.2727284542
Au	1.7657768595	2.8305145393	-0.1800606334
Au	-0.9740946389	2.2847094831	0.0539953154
Au	-0.7023972522	-3.2137271889	-0.0944909484
Au	1.7192702650	-4.3561731080	-0.3380887134
Au	-3.0896240397	-1.9805633838	-0.1541045932
Au	-0.0554670516	4.7855064397	-0.4032489523
Au	1.5892866333	-1.6966619595	0.1972813914
Sn	1.2117184326	0.7508464604	1.6144745531

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>11</sub>Si<sup>-</sup>

Isomer (a)

Au	-2.0374942967	-0.0006819643	-0.2545845306
Au	0.7071737237	-4.4521034094	1.1048209964
Au	-0.6377686371	2.3224676988	0.1670520525
Au	2.0280589519	2.1494044550	0.7046981571
Au	2.0296665537	-2.1488339358	0.7040109826
Au	-3.2473661294	-2.3866766685	-0.3709519262
Au	-0.6362725295	-2.3234296362	0.1663104251
Au	0.6709595079	-0.0002513345	-0.8630775762
Au	-3.2501808722	2.3840986298	-0.3645988739
Au	0.7051563097	4.4529807789	1.1023575034
Au	3.1694865708	0.0026397488	-2.1374968940
Si	2.9783175618	0.0007296447	0.2747724465

Isomer (b)

Au	-3.6104469708	-2.8686694776	-0.2622604232
Au	1.9172854046	4.1060395051	-0.6848736948
Au	0.4252961095	-2.8069123231	0.6555460731
Au	2.3153519606	1.4608382383	-0.4512231463
Au	2.9571119560	-3.6463655888	0.8940008213
Au	0.2156768586	-0.2149770209	-0.8424482477
Au	2.6405895287	-1.1171537669	0.0555256940
Au	-2.0216931486	-1.2275987459	-1.9061518397
Au	-0.1372857507	2.6322198471	0.1775880836
Au	-2.4038157067	3.2778590311	1.3933383348
Au	-2.0284993969	0.6774439498	0.9164536158
Si	-1.6660547788	-1.6562062090	0.5226099920

Isomer (c)

Au	-3.1070324228	1.4323290061	0.5629142024
Au	-1.0946193789	-2.7858905544	-0.3129279025
Au	0.7246116939	4.6923724110	-1.0281732182

Au	1.7723713295	2.2446977232	-1.1284397396
Au	-3.3009459944	-1.2827623438	0.0563570251
Au	1.6353315273	-2.4863584469	-0.4391383277
Au	3.0376191868	-0.7224922286	1.2813345533
Au	0.5651013623	-4.9152389877	-0.6175380255
Au	-0.8521364806	-0.1018037076	0.0922776216
Au	1.1227315155	1.2144853896	1.6118089556
Au	-0.7746185576	2.6995334673	0.0650019558
Si	1.5580423287	-0.0666252871	-0.5744618360

Isomer (d)

Au	1.4022465859	4.4766225656	-0.9341538723
Au	-3.0994980897	1.8503052303	0.1653442333
Au	3.8190918924	-0.6884233827	1.3861519689
Au	1.3431713986	-2.4591474790	-1.1592036240
Au	-0.8508539542	3.2119708373	-0.2779708077
Au	-1.1156543099	-2.2811237874	0.0907345369
Au	-0.4847475343	-4.3990279438	-1.4628703668
Au	-3.2146078131	-0.8490432159	0.9526739928
Au	-0.8180326858	0.4790945952	0.4143421094
Au	1.0908281905	-1.0825750364	1.4782145122
Au	1.5444685029	1.8088712517	-0.5453320614
Si	2.4028413379	-0.3965271517	-0.5734821798

Isomer (e)

Au	1.4235419775	1.5697965524	-0.8407357423
Au	2.7855192169	-0.7521585474	-0.8860614495
Au	-1.6169168435	0.0341225141	1.2012114320
Au	1.0462549949	-0.7247973364	1.3326213810
Au	-0.9778657924	-2.5349236288	0.1794431132
Au	0.1216115774	-0.7457148932	-1.6518097435
Au	-3.4951067214	-1.4245140057	-0.1917213770
Au	0.3540618316	3.9508628035	0.0067768983
Au	0.4026461635	1.8287889094	1.7761065870
Au	1.6773025900	-3.1087218693	0.1604185517
Au	-1.4097018061	2.0072055903	-0.8241493062
Si	-2.2518933524	-0.0873080774	-1.7883889070

The Cartesian coordinates of the top-five lowest-lying isomers of Au11Ge<sup>-</sup>

Isomer (a)

Au	-0.8492780736	4.9793478585	-0.4081157683
Au	-0.8882670583	-4.3225454266	-0.3248976254
Au	-1.4276351009	2.3739346480	0.1915030357

Au	1.2009797453	3.3112318727	-0.0990334509
Au	0.7424834416	0.6769852186	0.4662528054
Au	3.2534350128	1.5514955298	-0.0872952913
Au	1.8117370224	-3.7621545587	-0.3705938738
Au	0.0272462007	-1.8929817889	0.4394999809
Au	-2.6331859068	-2.1580389709	0.0240704677
Au	2.6909512407	-1.2038939064	0.0092716979
Au	-3.2974548608	0.4488409958	-0.4027669710
Ge	-1.5984606708	-0.0129839483	1.4362313622

Isomer (b)

Au	-0.7617905057	-1.3497556709	1.4877043277
Au	-2.7689757893	-0.0076857452	0.1455537486
Au	-0.7662533649	1.3412944175	1.4883000505
Au	-0.9163249181	-1.3390037706	-1.4462396154
Au	1.6842477052	-0.0022529606	1.9507975326
Au	-0.9240832548	1.3414738085	-1.4424105063
Au	-0.7149516334	-3.6620548272	0.0003478980
Au	-0.7233284646	3.6604800341	0.0111711435
Au	1.5061375712	0.0094527854	-2.0313501190
Au	1.5622682491	2.0657392788	-0.0540223786
Au	1.5666244912	-2.0601038400	-0.0656009595
Ge	3.1513073708	0.0045443498	-0.1019641119

Isomer (c)

Au	1.3870228605	-4.7626926368	-0.4499002978
Au	-0.4027409549	-2.8169204149	0.0654196422
Au	2.7371635789	3.1025603562	-0.0463700528
Au	-1.2372608818	-0.2177736882	0.3807591339
Au	-1.9434918829	2.4656039029	-0.1905180464
Au	2.2978290143	-2.2371549512	-0.1609860255
Au	2.9248930284	0.3438975348	-0.0839525389
Au	-3.0519659079	-2.1125362693	-0.0203487704
Au	0.5700379731	1.7165301360	0.5556266690
Au	-3.8498834151	0.5411858565	-0.1503962218
Au	0.1407168503	4.2170216159	-0.4899385679
Ge	1.0752177141	-0.6450166384	1.4913964205

Isomer (d)

Au	2.0835887541	-0.0022196477	0.2274896052
Au	-1.9644200960	2.1927938775	-0.6851478808
Au	-1.9682983404	-2.1906884046	-0.6795698689
Au	-0.6342892092	4.5025302908	-1.0151007978
Au	-0.6441240329	-4.5037836576	-1.0078595576

Au	-0.6319101420	-0.0001138147	0.8045877334
Au	0.7013123408	2.3326107521	-0.1666324343
Au	-3.0859173778	0.0084056220	2.1238454173
Au	3.3137653793	2.3758860043	0.3549971117
Au	3.3129284874	-2.3811446056	0.3460371666
Au	0.6985781368	-2.3352793074	-0.1666269795
Ge	-2.9888050396	0.0024471812	-0.3546704194

Isomer (e)

Au	2.1612638500	-4.4205962682	0.0022958150
Au	3.0534034547	3.5276116666	-0.1121354972
Au	-1.8968659042	1.3923278489	0.2483827306
Au	-2.5829322309	-2.4659186231	-0.6697970797
Au	2.5065877046	-1.7537956357	-0.0318644718
Au	-4.0805878015	-0.2673218113	0.0539287027
Au	-1.8213321073	4.0247506004	-0.2301028957
Au	0.2768942347	-0.2068852487	0.2742418321
Au	0.5206416918	2.7137743683	-0.0378577756
Au	-0.0852924841	-2.9995176394	0.0367828047
Au	2.7354339218	0.8722512953	-0.0782252299
Ge	-1.9292798588	-1.0374698314	1.3264201496

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>1</sub>1Sn<sup>-</sup>

Isomer (a)

Au	1.8512141002	-3.7367502612	-0.4543511775
Au	0.0582499188	-1.9177031966	0.4935763911
Au	3.2883273221	1.5266719844	-0.0882678812
Au	0.7663497453	0.6743012146	0.5519275288
Au	-0.7520703384	4.9894933984	-0.5399090644
Au	-3.2694657710	0.4610887286	-0.5074339668
Au	1.2422114949	3.2845977559	-0.1309605404
Au	-2.5892589198	-2.1589362737	-0.1110811293
Au	2.7130476022	-1.2041747833	0.0465989516
Au	-1.3992108393	2.3956003695	0.1238731803
Au	-0.8344815886	-4.3130417356	-0.4365082221
Sn	-1.7154671351	-0.0046986019	1.6862981414

Isomer (b)

Au	-0.5981575385	1.7260138818	-0.5834291125
Au	-2.2595788039	-2.3127823347	0.2629439544
Au	-2.7956501548	3.0202125562	0.1297635475
Au	3.8730999870	0.6771736976	0.1884032135
Au	-2.9161048521	0.2679423134	0.1239772190



Au	1.8982971460	2.5405376765	0.1935939673
Au	0.4849899483	-2.7473686234	-0.0160794916
Au	1.2982105034	-0.1431945851	-0.4401860075
Au	-1.1859022759	-4.7694988909	0.6039482117
Au	-0.2312166713	4.1984021724	0.5927035533
Au	3.1290784108	-1.9986230055	0.0408990682
Sn	-1.1086706347	-0.7519506129	-1.7485832259

Isomer (c)

Au	-1.8800811468	-4.9685183324	-0.2615031953
Au	-2.3523598019	-2.3483564563	0.0440473618
Au	0.6811170525	3.1987036200	-0.2801038302
Au	-2.1388525096	3.0004972571	-0.0227445510
Au	2.0513416047	0.9609025328	0.0245334860
Au	-2.5258682378	0.3606566679	0.0598543580
Au	0.4022190584	-3.5729181827	-0.1590449481
Au	-0.0862174797	-0.9091387412	0.0611316832
Au	-0.8349539830	5.3954374150	-0.4177843991
Au	2.4590846114	-1.8677647294	-0.0503873654
Au	4.5018181707	-0.1509420866	0.0239122145
Sn	-0.4370010130	1.4357401264	1.5597886577

Isomer (d)

Au	2.6692733696	1.5016882338	-0.0949781614
Au	0.1709871433	2.9724718380	-0.0606290650
Au	0.3674756354	-2.7998057730	-0.0375563832
Au	-2.4287778676	2.8019978704	-0.6025833831
Au	-2.0533012788	-3.9089285614	-0.3754661102
Au	0.3346602406	0.1429329007	0.2679083155
Au	2.8388716002	-3.8014362218	0.0099351422
Au	-1.9633630685	-1.2840289006	0.1911879640
Au	-4.0045349255	0.5600301588	-0.1012451312
Au	2.7094011437	-1.1351516982	-0.0569952618
Au	2.5488416813	4.1775801089	-0.1161659825
Sn	-1.8683935947	1.2363525674	1.5539381953

Isomer (e)

Au	0.1361733991	-5.3589468693	0.0491188558
Au	-3.1510934133	-1.1286186215	0.1929186135
Au	2.2393810341	2.4166125667	0.3577043310
Au	-1.6752725093	-3.3333264575	0.2361459888
Au	-2.6811736211	4.2218820251	0.0007409794
Au	-0.5355432566	-0.6330058162	-0.0837548612
Au	4.4730514144	0.9593133363	0.1716006459

Au	-0.1112525699	3.5929712854	0.3218815381
Au	-2.1187786951	1.5511704658	-0.0512762869
Au	2.1818832552	-0.4132526867	-0.0957222540
Au	1.0238702633	-2.8434766041	-0.1545916339
Sn	0.3481094202	1.5369071751	-1.5046152255

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>12</sub>Si<sup>-</sup>

Isomer (a)

Au	-0.2838734727	-0.7243443514	-0.2875366903
Au	3.5551752572	-0.4792933088	0.6967227282
Au	0.4342582431	1.8347503444	-0.3781794998
Au	-1.2791743465	3.8617490178	0.0789756831
Au	1.2668514336	-5.0753940026	0.0139823021
Au	-4.7007752359	0.2804156587	0.2302137999
Au	1.4367698863	4.3324811179	-0.0037812126
Au	-2.8040888962	-1.6124021083	0.1246053359
Au	3.1034062108	2.1295176139	0.0482808890
Au	-2.2418563092	1.2781163206	-0.0304563411
Au	1.9342192540	-2.4940569880	-0.2186604378
Au	-0.8007498831	-3.3620836408	0.0284108672
Si	2.0136926443	-0.0580828932	-1.1944771389

Isomer (b)

Au	0.2227480806	-3.1271956437	-0.3839131515
Au	2.0987984216	0.3333119884	1.8146371779
Au	-2.5064292719	0.7597172826	0.4659081139
Au	-2.0851720654	3.4323587818	0.9161068434
Au	-0.0699556078	1.8777977789	2.0020488307
Au	-0.0843119093	-0.4747764407	0.4187266302
Au	-2.4031474577	-1.8544273859	-0.0204378832
Au	3.8211672211	-1.6136887249	1.0306941540
Au	1.1022476593	2.8516074085	-2.9305396882
Au	-0.3083980969	2.2509280602	-0.7686064504
Au	-2.0753268736	-4.4791608828	-0.4925160183
Au	1.7638706021	0.5865906133	-1.6498879376
Si	2.0557698370	-1.5491245738	-0.6030907688

Isomer (c)

Au	4.5090066253	-1.1205806092	-0.7034871485
Au	2.1876290867	-2.4463746823	-0.5400556321
Au	2.4059145467	0.4113108206	-0.1117573865
Au	-0.0548576777	-4.8761630870	1.5479455630
Au	-4.5321158448	-1.0306054674	-0.6892002821
Au	0.0445811746	4.5483172518	0.3382330530

Au	-2.2362483305	-2.4013743085	-0.5354513839
Au	0.0179736752	1.7837989954	0.2079699110
Au	-2.3974005206	0.4581256336	-0.0997719620
Au	-0.0084121610	-0.9026377085	0.1474802295
Au	2.3628217113	3.1164744881	0.2226957577
Au	-2.3010482601	3.1609857632	0.2399854003
Si	-0.0343200729	-3.4226322120	-0.3111955591

Isomer (d)

Au	-1.8715439622	0.9914557613	0.9777514181
Au	-1.1763420182	-1.5190355518	1.7173889174
Au	1.3166384377	-2.3838461132	0.9281485337
Au	0.8910344331	0.3293142852	1.4646694579
Au	-2.2132411470	-1.0770335806	-0.9232274638
Au	2.7700692294	-0.5455075414	-0.5674256660
Au	2.7259531928	2.0711621106	0.2602214910
Au	0.1520377505	2.9030928385	0.6003202157
Au	0.7107772307	1.0769844152	-1.5535037862
Au	-1.0977090875	-3.5112246603	-0.2034645928
Au	-2.3573743653	3.1375548878	-0.6125418865
Au	0.4409434926	-1.6706441836	-1.6264609254
Si	-1.7035393977	1.1271938323	-1.8754300842

Isomer (e)

Au	-0.3347706672	0.6214501351	-0.4253268104
Au	-0.1159235742	-4.5139973215	0.1606011969
Au	2.0289257475	1.9676325581	-0.0199033817
Au	4.6697151694	1.7729153221	0.5219217902
Au	-2.7499556759	-3.4489050898	0.4314158558
Au	-2.6025313722	4.6428219573	0.0639524441
Au	3.3731608263	-0.5010547547	0.0073686815
Au	-2.7363551025	1.9489998470	0.1464180094
Au	2.0292744941	-2.8329755343	0.0662577974
Au	-0.2851160152	3.3047268668	-0.0961782352
Au	-0.6581453465	-2.0409336174	-0.6216662811
Au	-2.8452255535	-0.6981736877	0.2447565048
Si	1.3999305709	-0.9129760017	-1.4488282835

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>12</sub>Ge<sup>-</sup>

Isomer (a)

Au	2.8096185450	1.8101187806	-0.0275865355
Au	2.3049225067	-2.9944468926	-0.1121341454
Au	-0.0001865286	1.8794479055	0.1630317661
Au	1.3713677292	4.1748752519	-0.1879823347

Au	-2.3116229409	-2.9911713189	-0.1149569227
Au	1.3150040505	-0.4896218780	0.3394798941
Au	-2.8099160572	1.8140316141	-0.0299568884
Au	-0.0041125321	-4.4851162622	-0.4794039296
Au	-3.9290002954	-0.7080661371	-0.0672724687
Au	-1.3189329094	-0.4877248253	0.3378676582
Au	-1.3683225329	4.1768427215	-0.1915396956
Au	3.9251993963	-0.7135066953	-0.0619994094
Ge	-0.0040033661	-2.6332166717	1.2440140663

Isomer (b)

Au	-1.8630629552	-2.5138428099	0.1260639882
Au	-3.5966966819	-0.5561345355	-0.6319343873
Au	2.8649404264	-1.5613873401	-0.0767838168
Au	-3.1066126177	2.0672231843	-0.0378745465
Au	4.7375891979	0.3568121919	-0.1598773277
Au	1.2605526152	3.8925638644	-0.1388140886
Au	-0.4197989509	1.8332697075	0.3435644220
Au	0.8893471985	-3.3408579650	-0.0374064629
Au	2.2616203327	1.3229170180	0.0543866638
Au	-1.4615164514	4.2955226576	-0.0805777979
Au	-1.1473602302	-5.0844658328	-0.1189841232
Au	0.3261006230	-0.7148050914	0.3043373252
Ge	-2.0048587155	-0.0747332548	1.2818743952

Isomer (c)

Au	-2.7810186410	-0.0047656966	-0.7136799625
Au	-1.9071144222	-5.1236589209	-0.1317504633
Au	2.9800855884	0.0052400358	-0.0272665941
Au	2.8633371235	2.7821509906	-0.2423398525
Au	0.4813389497	4.0138891708	-0.1311916000
Au	-1.9076200543	2.4198076375	0.2056397641
Au	0.6310650756	-1.3432300607	0.4334711858
Au	0.4964598166	-4.0127221825	-0.1269649986
Au	2.8743895262	-2.7726844260	-0.2355111285
Au	-1.9260416152	5.1167813943	-0.1312241025
Au	-1.8985252436	-2.4264755515	0.2028749754
Au	0.6259599717	1.3452509386	0.4309687598
Ge	-1.4213004633	-0.0025671951	1.3977655074

Isomer (d)

Au	0.3350521090	-3.7783327754	-0.0963652515
Au	2.8836357910	-2.8693943888	-0.2598423397
Au	1.0548487331	4.0877167991	-0.1476574758

Au	-4.0229246512	2.9370486761	-0.3635377320
Au	-2.9624265307	0.4771240466	-0.1347605101
Au	-1.8528485116	-1.9243536118	0.1210218347
Au	0.9734882533	1.4668043389	0.3750899141
Au	3.2835201949	-0.0814428429	-0.0757790863
Au	3.3865233366	2.6152744473	-0.2546677090
Au	-2.1719213084	-4.6054559283	-0.2392219026
Au	0.8517902910	-1.1937390657	0.4465925061
Au	-1.3771239474	2.7863848199	0.0967000648
Ge	-1.0310955532	0.2290978116	1.5179476045

Isomer (e)

Au	-0.5038172394	2.2118448000	-0.7209212386
Au	3.1735380117	-0.7662742690	-1.0011862087
Au	0.5683947933	-0.1420328297	-1.6515477374
Au	-0.6647260164	-4.0057621404	0.7735132183
Au	-3.2880450693	2.0225363660	-0.6921991211
Au	0.4926854215	1.0460220398	1.8885667771
Au	-0.1007523476	-1.5390359452	1.8241374381
Au	1.2508519284	-2.5785744302	-0.4943448973
Au	-1.5394744071	-1.9142433910	-0.8387821552
Au	1.0546793437	3.6173582816	1.1401706925
Au	2.2542862135	1.6644075338	-0.3081298773
Au	-1.9604047080	0.2401119531	0.8687649347
Ge	-1.9565280191	0.3178747274	-2.0644904574

The Cartesian coordinates of the top-five lowest-lying isomers of Au<sub>12</sub>Sn<sup>-</sup>

Isomer (a)

Au	1.7038360073	3.3075687177	0.2204814966
Au	-3.9679818477	-0.1061728421	0.1949597715
Au	2.1371948988	-3.9014031522	0.1879522060
Au	0.3574937015	-1.9067163054	-0.2139421674
Au	1.2051630325	0.6709426128	-0.3859641747
Au	-0.5490604241	-4.4173521828	0.2113292144
Au	-2.8183979755	2.4391481878	0.2592753156
Au	-2.4054188678	-2.3730377376	0.0946968611
Au	-0.8424305103	4.3763319903	0.6423386475
Au	3.7138713199	1.3697324923	0.1225763625
Au	-1.3887355761	0.1724653943	-0.3622387521
Au	3.1014804160	-1.3151546377	0.0418832605
Sn	-0.5368197137	2.6880948794	-1.4612455382

Isomer (b)

Au	1.9314271295	3.9989647156	-0.6216804592
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Au	-3.8261330784	-0.0709270284	-0.0459355756
Au	-2.4353952081	2.3041573704	-0.0580516982
Au	0.2765955204	2.2119723666	0.5244761387
Au	-2.3484759850	-2.3924481003	-0.0642277029
Au	2.8564510191	1.4118329909	-0.0402502579
Au	-0.6281532638	-4.4180210504	-0.7710195547
Au	2.0776390455	-3.9262210152	-0.6244208171
Au	2.9075144504	-1.3081368699	-0.0396381574
Au	0.3578427815	-2.2019270582	0.5221062765
Au	-1.2165171026	-0.0234513446	0.7560531599
Au	-0.7908352454	4.3933174315	-0.7625303501
Sn	1.3659029431	0.0235654692	1.9612214653

Isomer (c)

Au	-2.2405233570	1.4418478350	0.0864246311
Au	-1.1283948798	3.9442898321	-0.2631689095
Au	3.1624325730	1.9292573735	-0.1319526774
Au	-2.9797402605	-1.3927120867	-0.0642842330
Au	-4.7669673314	0.6047418508	-0.1045425667
Au	3.5895090304	-0.7472324299	-0.6232783132
Au	-0.3908705601	-0.6914319184	0.3522070058
Au	1.6031732516	4.2141779993	-0.2387634933
Au	0.8102464137	-5.1395387790	-0.2685315552
Au	-1.0960329491	-3.2663048489	-0.0927079343
Au	0.4645912094	1.8309558263	0.3502359835
Au	1.7132334916	-2.6231274201	0.0082072715
Sn	2.0789204046	-0.1871536687	1.5622735138

Isomer (d)

Au	1.6473229470	-1.7459998875	0.1502840171
Au	2.0419595706	2.9812790248	0.0269160834
Au	-0.4033272923	-0.6098819326	1.9067954134
Au	-2.1027136132	3.3500542138	-0.1614012415
Au	-2.1905280418	0.6192187065	-0.1428754846
Au	2.1772511561	0.5253177474	-1.1824287185
Au	-0.1386485004	2.0076784285	-1.5071449548
Au	-0.0724356729	-3.3230310243	1.6024277508
Au	0.0929970568	-3.4507261879	-1.3538387711
Au	-1.9372326355	-2.0278362290	0.0015119835
Au	-0.2270255701	2.0557694928	1.4566110752
Au	-0.2383244631	-0.7591042237	-1.8427458502
Sn	2.1849033169	0.6269304949	1.6900904680

Isomer (e)

Au	3.2592513446-1.5901221797	0.5799031025
Au	-0.7964728060 -1.0120873515	-1.8773725787
Au	-2.1822531043 0.8699413478	0.0948209050
Au	1.6472969661 0.2599630883	-0.6616591461
Au	0.2088758148 1.8329759183	1.4572344298
Au	0.9457027401-0.7236356112	2.0364719740
Au	-1.7161587861 -1.7604506929	0.8190938009
Au	-0.3423441352 1.5875731303	-1.9904397524
Au	-1.2590301569 -3.6493386293	-1.2352091835
Au	1.5692589060 3.0667215274	-0.6574828978
Au	-1.2531034240 3.4750560230	-0.1718585333
Au	0.8685442307-2.4750740494	-0.1439716493
Sn	-1.5968400895 0.1695071696	2.7817155042