Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Understanding the bonding and aromaticity of $[Au_3\{C_4H_4(X)_4E\}_3]^-$ (X=CF_3, CN, BO; E= Si, Ge): a trinuclear gold superhalogens

Subhra Das[a,c], Swapan Sinha[a], Gourisankar Roymahapatra[a], Mesías Orozco-Ic,[b*] Gobinda Chandra De,[c*] Santanab Giri[a*]

[a]School of Applied Science and Humanities, Haldia Institute of Technology, ICARE Complex, West Bengal 721657, India.

[b]Donostia International Physics Center (DIPC), 20018 Donostia, Euskadi, Spain.

[c]Department of Chemistry, Cooch Behar PanchananBarma University, Cooch Behar, 736101, West Bengal, India.

Corresponding Author Email: mesias.orozco@dipc.org, degobinda@yahoo.com, santanab.giri@gmail.com,

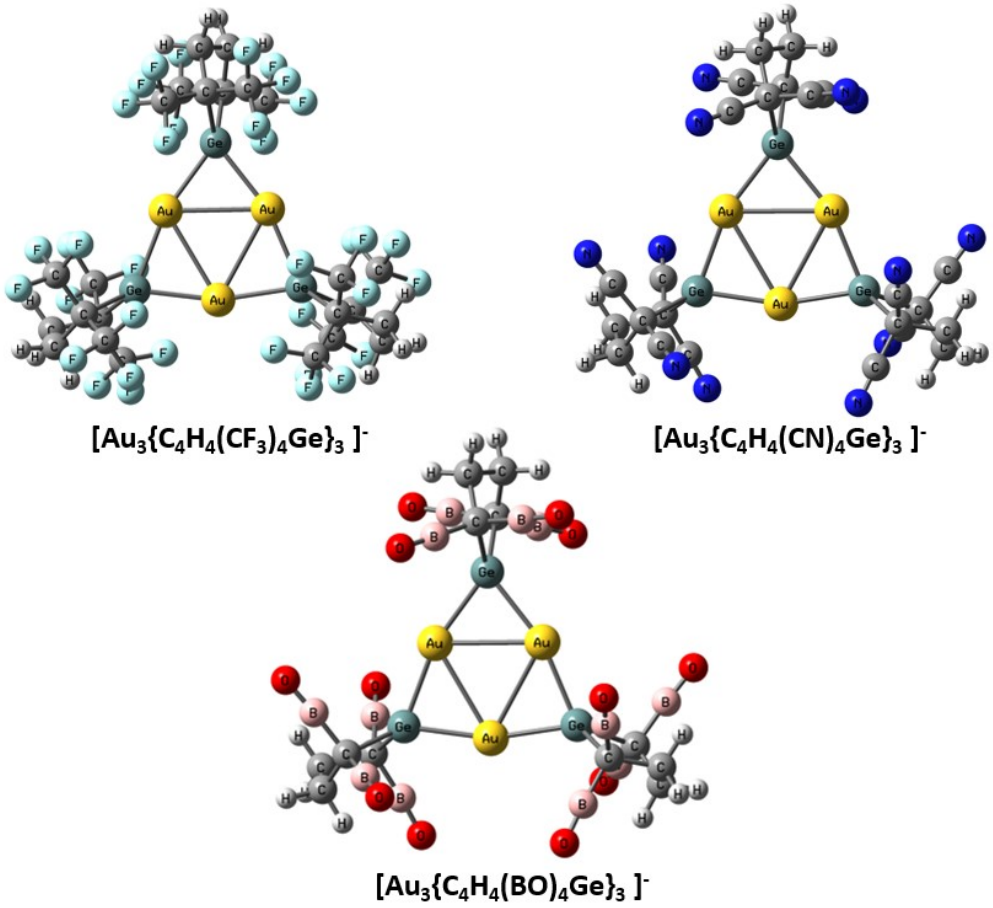


Fig S1: Optimized geometries of $[Au_3\{C_4H_4(CF_3)_4Ge\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$, $[Au_3\{C_4H_4(BO)_4Ge\}_3]^-$ complexes.

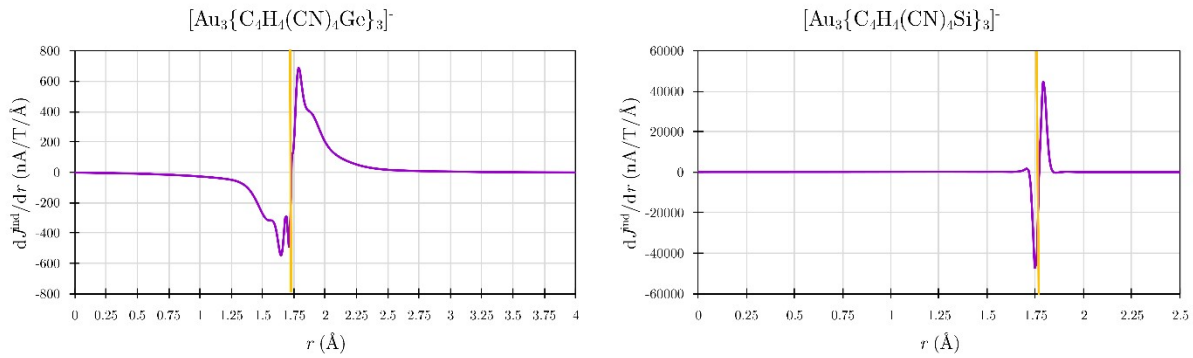


Fig S2: Ring-current profile for $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$ and $[Au_3\{C_4H_4(CN)_4Si\}_3]^-$. The vertical yellow line corresponds to the intersection of the integration plane with the Au nucleus. The abrupt sharp peaks of the curves correspond to the atomic circulations near the nuclei. Since the dia- and paratropic contributions of these atomic currents cancel each other near the intersection, when integrating the area under the curve, the remaining quantity is a good approximation of the ring-current strength.

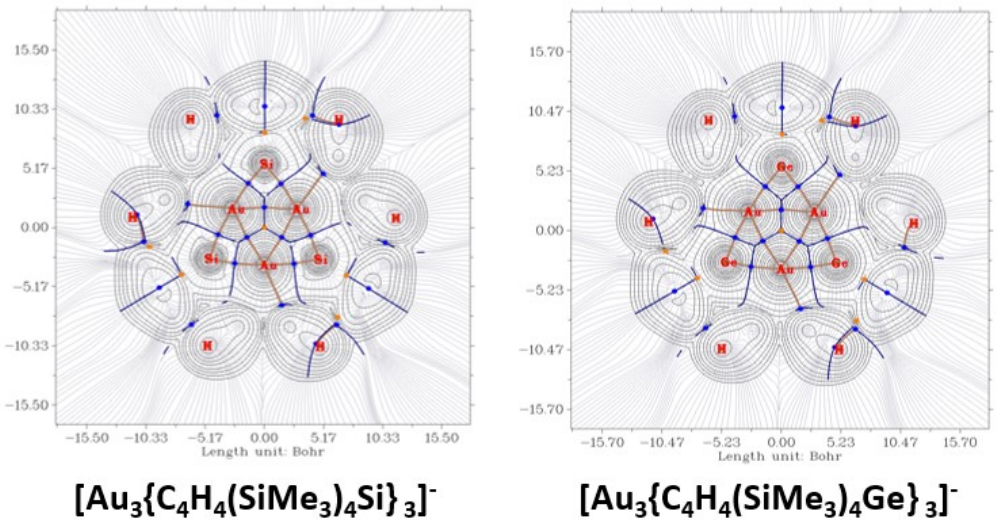


Fig S3: Contour plot of the Laplacian of the electron density along with bond path and bond critical points of $[Au_3\{C_4H_4(SiMe_3)_4Si\}_3]^-$, $[Au_3\{C_4H_4(SiMe_3)_4Ge\}_3]^-$.

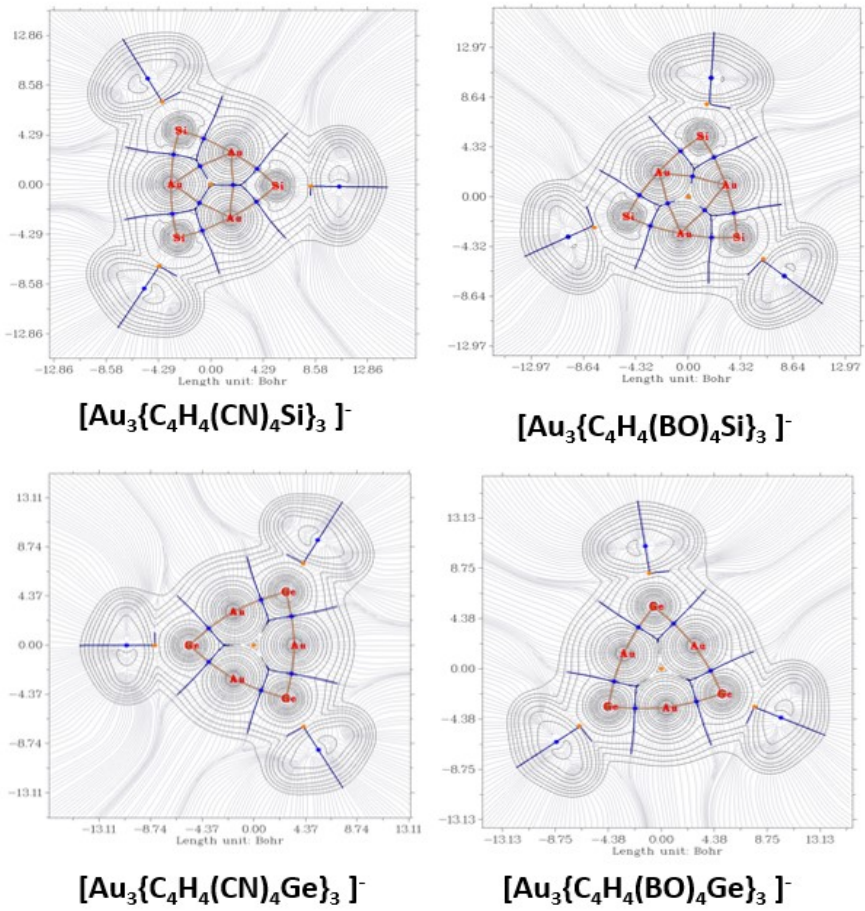


Fig S4: Contour plot of the Laplacian of the electron density along with bond path and bond critical points of $[Au_3\{C_4H_4(CN)_4Si\}_3]^-$, $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$ and $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$

Table S1: Calculated AIM parameters at BCP (3, -1) of $[Au_3\{C_4H_4(CN)_4Si\}_3]^-$, $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$and $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$ respectively.

Complex	BCP	ρ	Laplacian electron density ($\nabla^2\rho\ (r)$)	$-G_{CP}/V_{CP}$
$[Au_3\{C_4H_4(CN)_4Si\}_3]^-$	Au_1-Au_2	0.039	0.066	0.778
	Au_2-Au_{21}	0.039	0.065	0.778
	Au_{21}-Au_1	0.038	0.066	0.778
	Au_1-Si_3	0.072	-0.0026	0.491
	Au_1-Si_{22}	0.072	-0.0026	0.491
	Au_2-Si_3	0.072	-0.0025	0.491
	Au_2-Si_4	0.072	-0.0027	0.491

	Au_{21}-Si_4	0.072	-0.0027	0.491
	Au_{21}-Si_{22}	0.072	-0.0025	0.491
$[Au_3\{C_4H_4(BO)_4Si\}_3]^-$	Au_1-Au_2	0.392	0.0652	0.794
	Au_2-Au_{21}	0.393	0.0652	0.791
	Au_{21}-Au_1	0.393	0.0653	0.788
	Au_1-Si_3	0.072	-0.0037	0.482
	Au_1-Si_{22}	0.072	-0.0036	0.482
	Au_2-Si_3	0.072	-0.0039	0.482
	Au_2-Si_4	0.072	-0.0035	0.482
	Au_{21}-Si_4	0.072	-0.0039	0.482
	Au_{21}-Si_{22}	0.072	-0.0038	0.482
$[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$	Au_1-Ge_{53}	0.063	0.0563	0.556
	Au_1-Ge_{54}	0.063	0.0563	0.556
	Au_2-Ge_{52}	0.063	0.0563	0.556
	Au_2-Ge_{53}	0.063	0.0565	0.556
	Au_{19}-Ge_{52}	0.063	0.0563	0.556
$[Au_3\{C_4H_4(BO)_4Ge\}_3]^-$	Au_1-Ge_{53}	0.063	0.0555	0.556
	Au_1-Ge_{54}	0.063	0.0555	0.556
	Au_2-Ge_{52}	0.063	0.0576	0.556
	Au_2-Ge_{53}	0.063	0.0557	0.556
	Au_{19}-Ge_{52}	0.063	0.0558	0.556

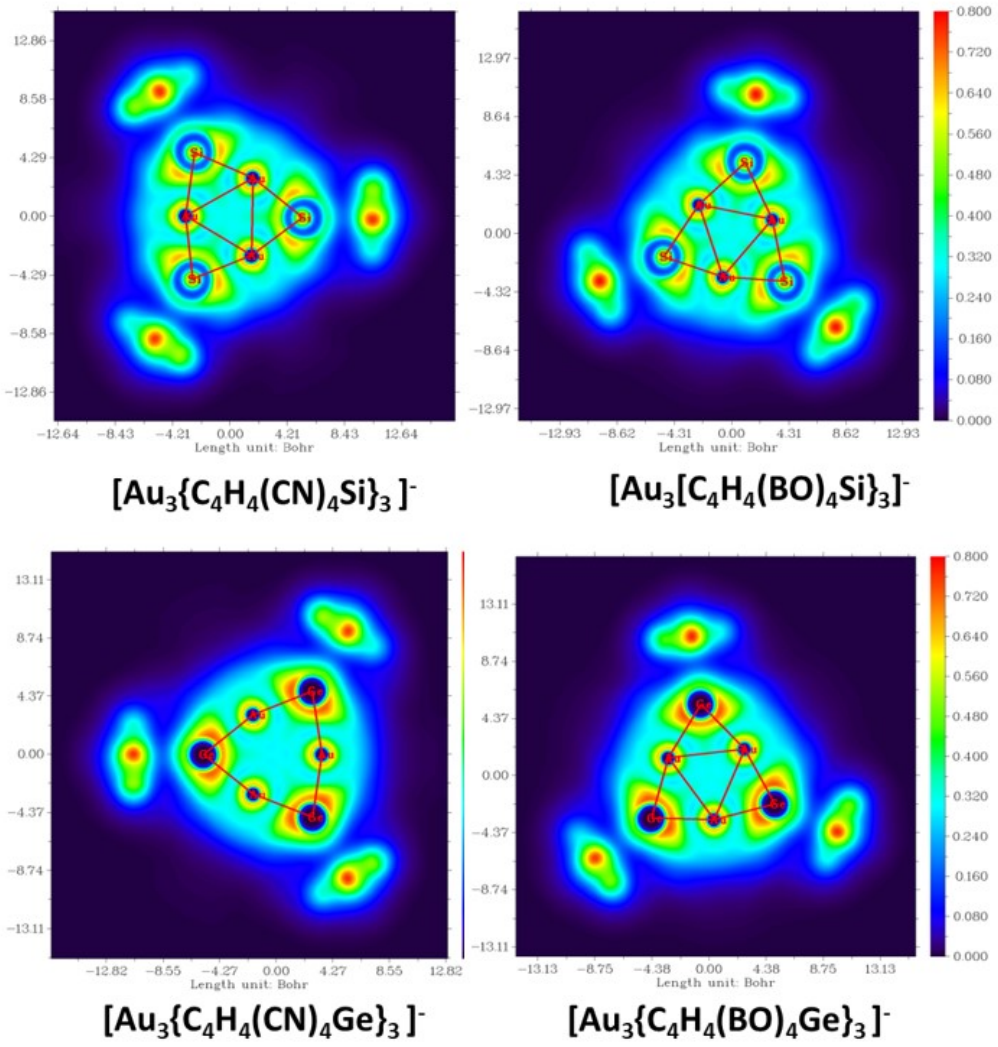
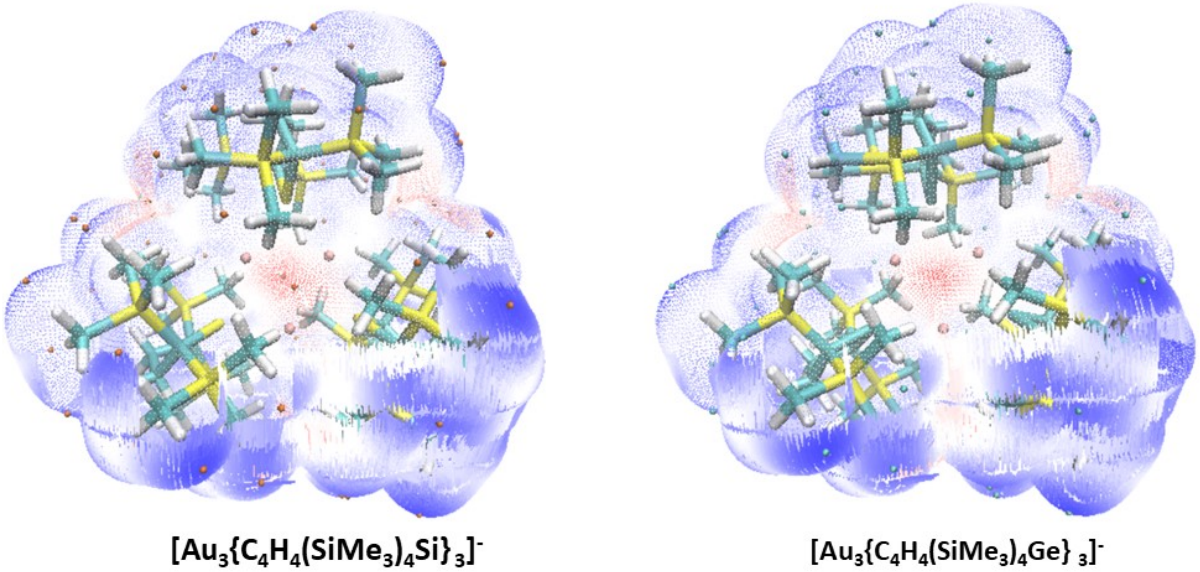


Fig S5: Cut of plane ELF plot of $[Au_3\{C_4H_4(CN)_4Si\}_3]^-$, $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$ and $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$.



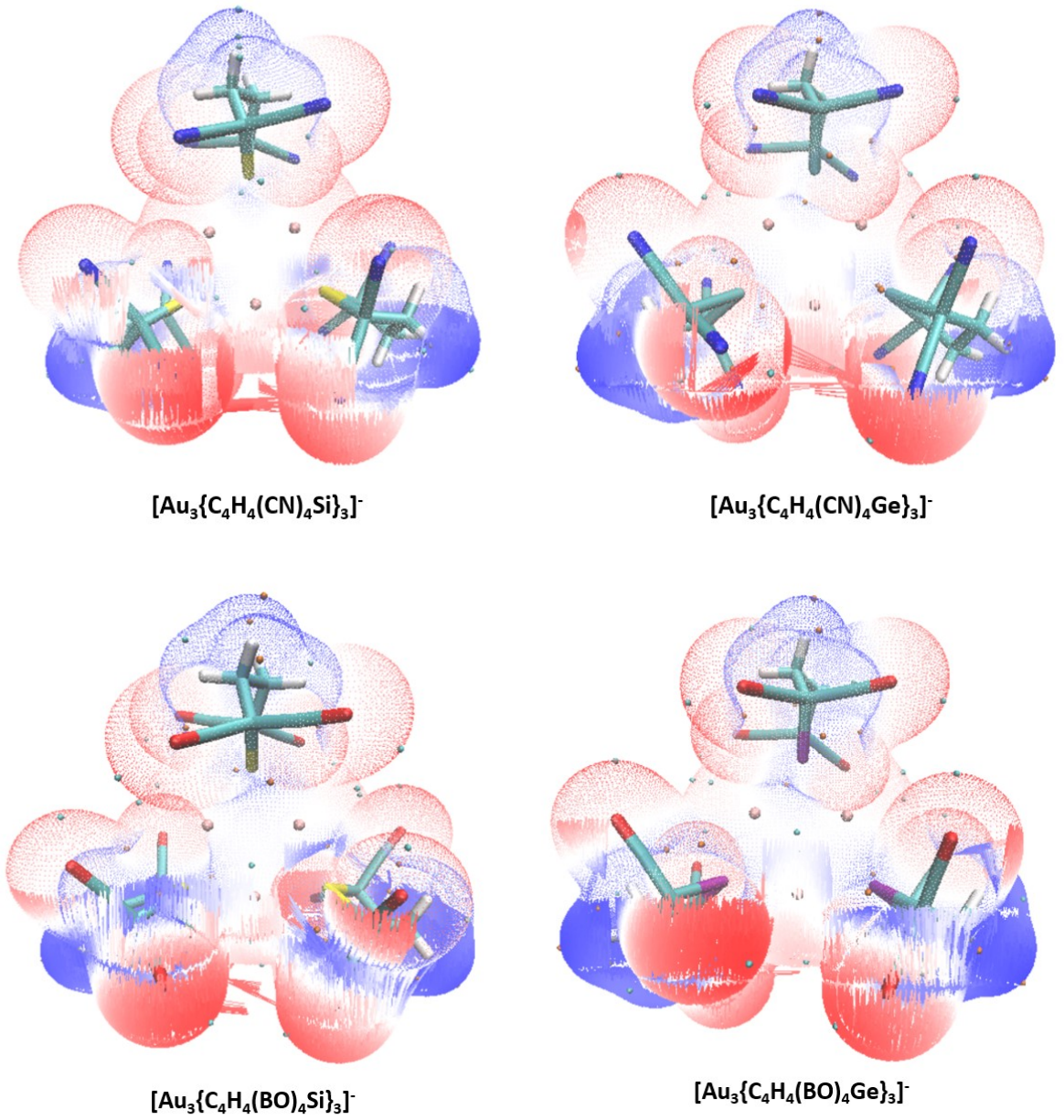


Fig S6: Molecular electrostatic potential map (MEP) of $[Au_3\{C_4H_4(SiMe_3)_4Si\}_3]^-$, $[Au_3\{C_4H_4(SiMe_3)_4Ge\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Si\}_3]^-$, $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$, and $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$.

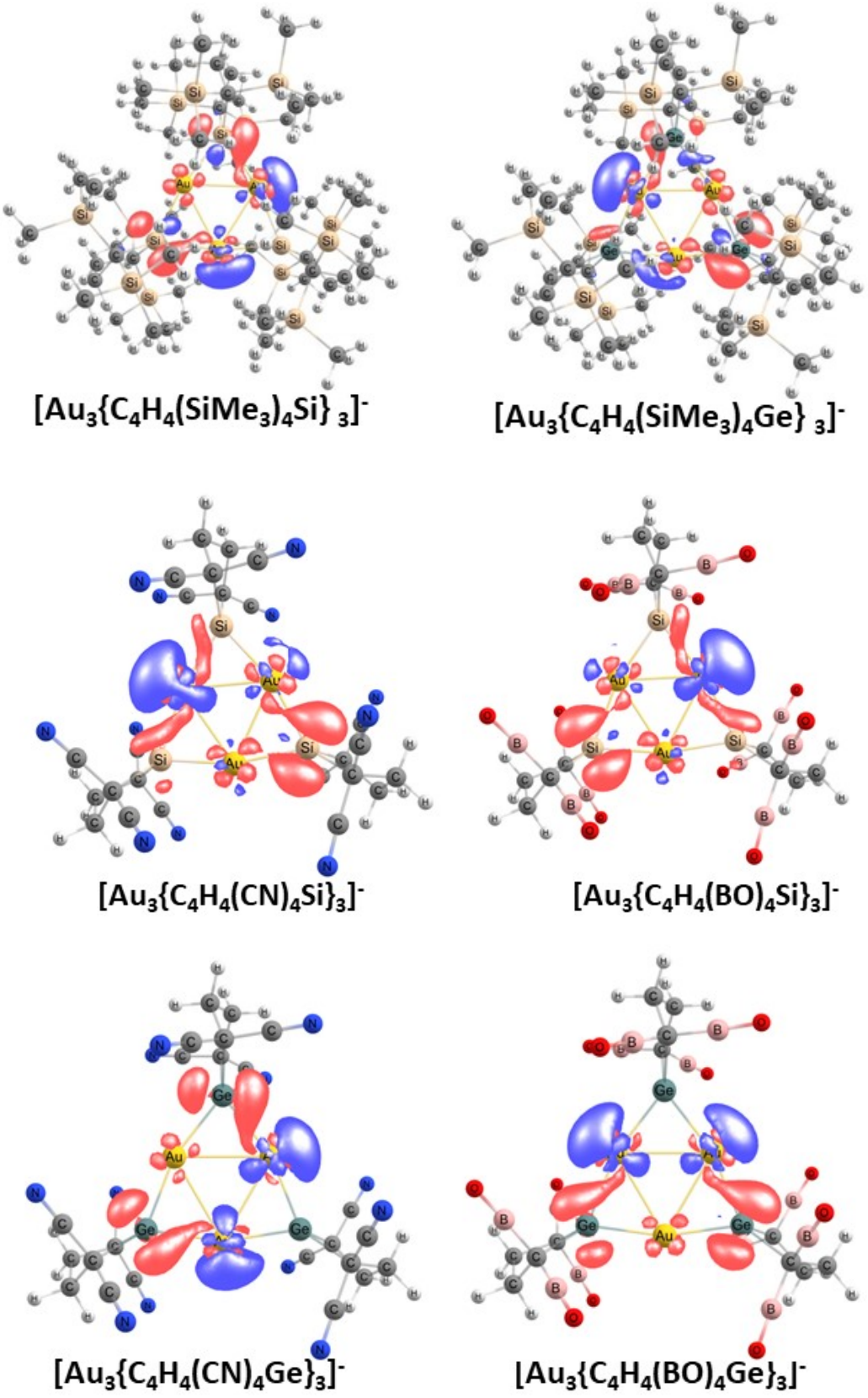


Fig S7: Calculated dual descriptor of $[Au_3\{C_4H_4(SiMe_3)_4Si\}_3]^-$, $[Au_3\{C_4H_4(SiMe_3)_4Ge\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Si\}_3]^-$, $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$, $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$ and $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$.

Table S2: Cartesian coordinates of optimized geometries of $[Au_3\{C_4H_4(CF_3)_4Si\}_3]^-$

Au	0.9335500	4.6133930	-3.7470870
Au	-0.4985320	4.6714100	-1.3411220
Si	-1.4397320	4.6660800	-3.5582910
Si	0.9324150	4.6157240	0.5894460
C	0.7963190	3.1920200	1.9431530
C	-2.5699450	3.2451180	-4.3095260
C	-2.5431470	6.1035360	-4.3144610
C	0.5836600	3.9383000	3.2799120
H	-0.4862080	4.0825380	3.4166420
H	0.9297290	3.3347950	4.1208890
C	-3.8212850	5.3968620	-4.8208370
H	-4.5362890	5.3706240	-4.0004200
H	-4.2870210	5.9666450	-5.6267740
C	-3.5270600	3.9699350	-5.2834830
H	-3.0522890	3.9981170	-6.2618670
H	-4.4575160	3.4118190	-5.3990330
C	1.0682230	6.0413480	1.9411460
C	1.2818330	5.2967410	3.2786820
H	2.3518270	5.1524320	3.4144930
H	0.9367690	5.9014110	4.1192410
Au	2.3642970	4.5576530	-1.3402350
Si	3.3068000	4.5620570	-3.5567300
C	4.4364470	5.9834380	-4.3079790
C	4.4114850	3.1250030	-4.3117470
C	5.6890920	3.8322730	-4.8186550
H	6.4042720	3.8592620	-3.9984210
H	6.1549980	3.2624840	-5.6244870
C	5.3938980	5.2588460	-5.2817760
H	4.9190000	5.2300080	-6.2600870
H	6.3239770	5.8175220	-5.3976740
C	2.2719160	6.9521170	1.6853310

C	-0.4080330	2.2817390	1.6887940
C	-0.2178860	6.8705000	1.9989540
C	2.0820730	2.3623890	2.0018980
C	-2.9274260	7.1354500	-3.2533600
C	-3.3704350	2.5466830	-3.2082830
C	-1.7327160	2.2244660	-5.0859640
C	-1.8165120	6.7833850	-5.4795490
C	5.2365610	6.6823950	-3.2067740
C	3.5988990	7.0036240	-5.0846910
C	3.6853680	2.4437180	-5.4763120
C	4.7965180	2.0942100	-3.2498430
F	4.3583650	7.9538030	-5.6687110
F	2.7096230	7.6394040	-4.3190550
F	2.9226850	6.4128830	-6.0799190
F	6.1205890	7.5786030	-3.6909270
F	4.4252920	1.4810440	-6.0623680
F	2.5331550	1.8746170	-5.1247990
F	3.4133680	3.3356240	-6.4460940
F	4.4727510	7.3333890	-2.3308760
F	5.9670710	5.7883280	-2.5149120
F	3.7476920	1.4199910	-2.7740460
F	5.6716710	1.1790320	-3.7166570
F	5.4034090	2.6818310	-2.2082370
F	-3.8018160	8.0509830	-3.7209080
F	-3.5348810	6.5490740	-2.2113880
F	-1.8781080	7.8091860	-2.7779800
F	-4.2548840	1.6508380	-3.6923370
F	-2.4924630	1.2743550	-5.6697270
F	-0.8436280	1.5886110	-4.3201640
F	-2.6069500	1.8954090	-2.3322940
F	-4.1005220	3.4412010	-2.5165700
F	-2.5558560	7.7459250	-6.0665670
F	-0.6640380	7.3521590	-5.1283910

F	-1.5448770	5.8904900	-6.4485350
F	-1.0563110	2.8147430	-6.0813370
F	3.4121270	6.2494530	1.6383440
F	2.4425170	7.8589920	2.6712730
F	2.1787920	7.6375440	0.5433140
F	-0.1959450	7.8022820	2.9745670
F	-1.2761900	6.0855370	2.2708140
F	-0.4852230	7.5177160	0.8646900
F	3.1404210	3.1472170	2.2741270
F	2.0593200	1.4309880	2.9778510
F	-0.5796990	1.3770230	2.6765230
F	-0.3152280	1.5939890	0.5481360
F	2.3499370	1.7146100	0.8680890
F	-1.5476330	2.9852780	1.6401380

Table S3: Cartesian coordinates of optimized geometries of $[Au_3\{C_4H_4(CN)_4Si\}_3]^-$

Au	-1.2227100	1.1106290	5.3719680
Au	-2.6587330	1.1079400	7.8343400
Si	-3.5958570	1.1527370	5.6321450
Si	-1.2244020	1.1126710	9.7511000
C	-1.1749940	-0.3003700	11.1236020
C	-4.8293230	-0.1970340	4.9004680
C	-4.7055390	2.6286420	4.9409960
C	-1.5737450	0.4376550	12.4278940
H	-2.6580090	0.5699570	12.4302420
H	-1.3076190	-0.1549080	13.3036210
C	-6.0398330	1.9404890	4.5525410
H	-6.6224440	1.7820170	5.4628260
H	-6.6251350	2.5771260	3.8885740
C	-5.7020420	0.6080310	3.9017670
H	-5.1232530	0.7649420	2.9887740
H	-6.5994610	0.0484730	3.6363380
C	-1.2739590	2.5261340	11.1231110
C	-0.8747370	1.7885950	12.4275270

H	0.2095330	1.6563080	12.4295080
H	-1.1405380	2.3814740	13.3031400
Au	0.2111720	1.1163640	7.8354200
Si	1.1503360	1.0694450	5.6343290
C	2.3831740	2.4189260	4.9012760
C	2.2613840	-0.4067800	4.9459410
C	3.5946630	0.2818000	4.5547270
H	4.1783760	0.4419400	5.4640070
H	4.1795310	-0.3553510	3.8908760
C	3.2552210	1.6131660	3.9025680
H	2.6754140	1.4546950	2.9904810
H	4.1519700	2.1729530	3.6353480
C	-2.0818400	-1.3952300	10.8064620
N	-2.8180410	-2.2435840	10.5734140
C	0.1947610	-0.7961340	11.2435110
N	1.2814500	-1.1350860	11.3901020
C	-2.6437990	3.0216210	11.2431130
N	-3.7305630	3.3603210	11.3897360
C	-0.3673880	3.6210590	10.8054120
N	0.3686540	4.4694320	10.5719320
C	3.2297460	2.9319690	5.9763960
N	3.9469290	3.2830630	6.8006890
C	1.6708550	3.5120460	4.2529800
N	1.1137690	4.3577810	3.7141870
C	2.4476000	-1.4503390	5.9455960
N	2.6148650	-2.2573640	6.7435630
C	1.6304120	-0.9601860	3.7496280
N	1.1769740	-1.3486750	2.7695690
C	-4.1174880	-1.2906180	4.2524140
N	-3.5607750	-2.1366980	3.7137760
C	-5.6752220	-0.7093280	5.9764770
N	-6.3919270	-1.0599100	6.8014000
C	-4.8898320	3.6749500	5.9381010

N	-5.0556110	4.4842720	6.7340490
C	-4.0750750	3.1781780	3.7426230
N	-3.6222990	3.5634100	2.7609690

Table S4: Cartesian coordinates of optimized geometries of $[Au_3\{C_4H_4(BO)_4Si\}_3]^-$

Au	-1.1454430	-0.3434450	5.2711830
Au	-2.8005370	-0.2859860	7.7330610
Si	-3.4042780	0.3550950	5.5121890
Si	-1.4376120	0.3119990	9.5849740
C	-1.4420810	-0.1499460	11.4784040
C	-5.0634820	-0.0569540	4.5761110
C	-3.7024230	2.2699500	5.3548460
C	-1.3495960	1.2098660	12.2462760
H	-2.3572920	1.5653740	12.4734040
H	-0.8264720	1.0954210	13.1967500
C	-5.2555120	2.3425130	5.3087430
H	-5.6581050	2.1057720	6.2983030
H	-5.6026500	3.3434250	5.0459800
C	-5.7465150	1.3210560	4.2852390
H	-5.4694240	1.6555900	3.2829580
H	-6.8339820	1.2383980	4.3086000
C	-1.3497840	2.2175080	9.9665420
C	-0.6457150	2.2296460	11.3536610
H	0.4068730	1.9570830	11.2293940
H	-0.6740150	3.2208730	11.8096350
Au	0.1616590	-0.3667590	7.9452140
Si	1.1054930	0.2211980	5.8429960
C	1.4676550	2.1224300	5.6264650
C	2.7261440	-0.2777730	4.8818890
C	3.4077360	1.0685080	4.4698530
H	4.1147220	1.3682620	5.2467600
H	3.9723160	0.9609270	3.5425840
C	2.3283100	2.1398800	4.3305150
H	1.6924750	1.9206330	3.4672760
H	2.7796640	3.1194530	4.1631940
O	-0.9571450	3.3054850	5.2265310

O	3.2279070	2.8513600	7.5694250
O	2.0033470	-1.6838800	2.6514190
O	4.3011600	-1.8489810	6.4679470
O	-2.7589380	3.3750180	7.6617350
O	-6.6152500	-1.5823580	6.2308770
O	-4.5066910	-1.4885120	2.3166750
O	-2.9208300	3.0221970	2.8573930
O	0.2478010	3.3047820	8.0408430
O	-3.8669810	3.1040650	10.5080050
O	0.7762390	-1.6641150	11.9884920
O	-3.6845530	-1.5870270	12.0877450
B	-0.5458940	2.8697020	8.8484940
B	-2.7833260	2.7574930	10.1040950
B	-0.2049060	-1.0136050	11.7328720
B	-2.6968860	-0.9574100	11.8073220
B	0.1240640	2.8267000	5.4977300
B	2.3186660	2.5845930	6.8212850
B	2.2954330	-1.0796240	3.6518150
B	3.5978780	-1.1590200	5.7753540
B	-3.0872660	2.9303950	6.5818270
B	-3.1106150	2.7364860	4.0148220
B	-5.9066720	-0.9230680	5.5136740
B	-4.7421230	-0.8605760	3.3168240

Table S5: Cartesian coordinates of optimized geometries of $[Au_3\{C_4H_4(CF_3)_4Ge\}_3]^-$

Au	0.935075000	4.339784000	-3.836105000
Au	-0.514111000	4.549606000	-1.357335000
C	0.773234000	3.123734000	2.085843000
C	-2.865198000	3.221595000	-4.327691000
C	-2.530241000	6.112983000	-4.409942000
C	0.603703000	3.923242000	3.393175000
H	-0.460240000	4.089225000	3.549916000
H	0.957862000	3.342435000	4.247218000
C	-3.878243000	5.505687000	-4.846444000
H	-4.561270000	5.561280000	-4.001226000
H	-4.323943000	6.094910000	-5.650116000

C	-3.740005000	4.046886000	-5.291786000
H	-3.276154000	4.013954000	-6.275549000
H	-4.729560000	3.597281000	-5.395231000
C	1.095455000	6.019353000	2.021622000
C	1.324960000	5.270664000	3.349464000
H	2.395317000	5.107358000	3.459735000
H	1.013758000	5.885876000	4.196206000
Au	2.394779000	4.411907000	-1.352119000
C	4.420817000	6.028112000	-4.366207000
C	4.711577000	3.132874000	-4.386915000
C	5.889669000	4.002974000	-4.868812000
H	6.587931000	4.113125000	-4.041898000
H	6.431856000	3.503253000	-5.673773000
C	5.434175000	5.387622000	-5.335747000
H	4.957308000	5.301594000	-6.310241000
H	6.301971000	6.036892000	-5.467706000
C	2.298625000	6.916291000	1.738911000
C	-0.465450000	2.259350000	1.865757000
C	-0.189903000	6.842314000	2.078384000
C	2.032420000	2.262526000	2.141858000
C	-2.759699000	7.201546000	-3.364159000
C	-3.703927000	2.674766000	-3.175881000
C	-2.183669000	2.082484000	-5.081286000
C	-1.782789000	6.671371000	-5.619539000
C	5.148250000	6.764838000	-3.244386000
C	3.504232000	6.975529000	-5.138297000
C	4.084213000	2.387003000	-5.562096000
C	5.185118000	2.156960000	-3.314347000
F	4.188095000	7.969621000	-5.744685000
F	2.582036000	7.556184000	-4.367806000
F	2.855864000	6.327076000	-6.117021000
F	5.940894000	7.755802000	-3.700459000
F	4.966632000	1.599548000	-6.210603000
F	3.064164000	1.603561000	-5.210625000
F	3.623800000	3.254876000	-6.481662000

F	4.329839000	7.311218000	-2.345886000
F	5.962386000	5.922685000	-2.579239000
F	4.190988000	1.430040000	-2.797241000
F	6.104925000	1.285570000	-3.779834000
F	5.771696000	2.805670000	-2.296905000
F	-3.499752000	8.224778000	-3.839762000
F	-3.432435000	6.720355000	-2.308103000
F	-1.624487000	7.729612000	-2.901018000
F	-4.706674000	1.875720000	-3.592931000
F	-3.071494000	1.217929000	-5.616831000
F	-1.363776000	1.362245000	-4.309888000
F	-2.995096000	1.967128000	-2.296238000
F	-4.293979000	3.679385000	-2.501358000
F	-2.480645000	7.626698000	-6.267964000
F	-0.600060000	7.203571000	-5.315483000
F	-1.564670000	5.701565000	-6.527742000
F	-1.457502000	2.547066000	-6.107583000
F	3.429616000	6.199451000	1.668303000
F	2.498462000	7.822198000	2.720545000
F	2.189678000	7.601324000	0.598411000
F	-0.164247000	7.784650000	3.043921000
F	-1.243766000	6.055959000	2.364486000
F	-0.467478000	7.474224000	0.937737000
F	3.112556000	3.022211000	2.403679000
F	1.989858000	1.336120000	3.122015000
F	-0.682597000	1.409987000	2.893065000
F	-0.401110000	1.517126000	0.757327000
F	2.279132000	1.602605000	1.009337000
F	-1.571318000	3.012589000	1.778515000
Ge	0.938357000	4.541755000	0.618426000
Ge	3.366423000	4.453694000	-3.604741000
Ge	-1.489830000	4.549260000	-3.609226000

Table S6: Cartesian coordinates of optimized geometries of $[Au_3\{C_4H_4(CN)_4Ge\}_3]^-$

Au	-0.6897690	0.3706150	-2.4436850
Au	-2.1608180	0.3849520	0.0870540
C	-0.6740010	-1.0705750	3.5075600

C	-4.4395040	-0.9717920	-2.8971720
C	-4.3247560	1.9168770	-2.8844910
C	-1.0581600	-0.2916380	4.7872370
H	-2.1387720	-0.1315230	4.7813950
H	-0.8149610	-0.8745170	5.6766690
C	-5.6476940	1.1874070	-3.2152410
H	-6.1967490	1.0331260	-2.2834330
H	-6.2697670	1.8015330	-3.8676380
C	-5.3231080	-0.1499750	-3.8649050
H	-4.7667720	0.0029050	-4.7925160
H	-6.2325980	-0.6995370	-4.1113240
C	-0.7094850	1.8192320	3.5053830
C	-0.3259080	1.0422470	4.7864050
H	0.7547100	0.8821570	4.7813260
H	-0.5695520	1.6264550	5.6748450
Au	0.7795100	0.3592600	0.0881330
C	3.0583660	1.7160250	-2.8960170
C	2.9470730	-1.1727580	-2.8813070
C	4.2688430	-0.4419040	-3.2136910
H	4.8185200	-0.2863520	-2.2824650
H	4.8910780	-1.0557420	-3.8662030
C	3.9421720	0.8946810	-3.8639460
H	3.3852640	0.7405920	-4.7910210
H	4.8508240	1.4451580	-4.1114200
C	-1.6128090	-2.1353490	3.1971700
N	-2.3790860	-2.9572370	2.9642820
C	0.6832520	-1.5890960	3.6217490
N	1.7675520	-1.9403980	3.7593580
C	-2.0667940	2.3379050	3.6181730
N	-3.1511610	2.6893840	3.7548020
C	0.2294780	2.8835160	3.1937810
N	0.9958890	3.7050050	2.9599330
C	3.8613180	2.2155090	-1.7871080
N	4.5422760	2.5523010	-0.9264610
C	2.3572970	2.8016120	-3.5606230
N	1.7999850	3.6396480	-4.1119180
C	3.1182130	-2.2168720	-1.8845870
N	3.2726800	-3.0216620	-1.0812290
C	2.3470650	-1.7078660	-4.0965200
N	1.9105700	-2.0771410	-5.0919730
C	-3.7395260	-2.0580640	-3.5618070
N	-3.1830220	-2.8966380	-4.1131010
C	-5.2423870	-1.4704030	-1.7878210
N	-5.9232520	-1.8064910	-0.9268250
C	-4.4939900	2.9625650	-1.8891040
N	-4.6470120	3.7686820	-1.0868020
C	-3.7246950	2.4494810	-4.1007850
N	-3.2883150	2.8167530	-5.0970320
Ge	-0.6913320	0.3732400	2.0452990
Ge	-3.1171830	0.4191010	-2.1656090
Ge	1.7375070	0.3241630	-2.1638340

Table S7: Cartesian coordinates of optimized geometries of $[Au_3\{C_4H_4(BO)_4Ge\}_3]^-$

Au	-1.2987920	2.6826490	5.1909710
Au	-2.6708060	2.7092610	7.9687120
C	-1.1116720	0.0056820	10.0094790
C	-3.9669570	0.0992300	5.6105820

C	-5.2963670	2.5018510	4.7320890
C	-1.7975680	-0.0192200	11.3999190
H	-2.8509700	0.2585650	11.2948420
H	-1.7694880	-1.0192490	11.8373740
C	-5.9387000	1.1093460	4.4489480
H	-6.6067570	0.8427350	5.2714900
H	-6.5425050	1.1349470	3.5400110
C	-4.8415070	0.0525410	4.3307830
H	-4.2215840	0.2549730	3.4518140
H	-5.2867510	-0.9347180	4.1924520
C	-1.0271290	2.3758440	11.6450560
C	-1.0848610	0.9712960	12.3202200
H	-0.0681490	0.6172840	12.5070010
H	-1.5884320	1.0225550	13.2870560
Au	0.3925600	2.6266680	7.7522400
C	2.8133030	2.2514530	4.5599390
C	1.2676920	-0.0548610	5.3258960
C	2.8110260	-0.1796040	5.2472830
H	3.2470800	0.0285460	6.2293630
H	3.1123300	-1.1914270	4.9688890
C	3.3359700	0.8212930	4.2198650
H	2.9839010	0.5327920	3.2264280
H	4.4268410	0.8014950	4.1904360
O	2.4414250	3.8112660	2.3521300
O	4.4541750	3.4433350	6.3890250
O	0.4031980	-0.7485210	2.8418540
O	0.2952850	-1.0652800	7.6623270
O	-6.8759520	4.1486390	6.2287980
O	-5.7066390	-0.5576490	7.5930380
O	-1.5077590	-1.0144710	5.2375650
O	-4.5303140	3.6532030	2.3775140
O	1.2044440	3.8185170	12.2711460
O	-3.2768110	3.8244020	12.1943200
O	1.4173150	-0.8649530	10.5048150
O	-2.7217850	-1.0054480	8.0551740
B	0.2194050	3.1842160	11.9897160
B	-2.2797460	3.2009850	11.9309380
B	0.3261950	-0.5222910	10.1169780
B	-1.9254070	-0.6040560	8.8777730
B	2.6018500	3.1297310	3.3325990
B	3.7096670	2.9416760	5.5853660
B	0.6273380	-0.4852660	3.9988860
B	0.6402560	-0.6624240	6.5708730
B	-6.1733450	3.4288890	5.5652080
B	-4.8505450	3.1730630	3.4354970
B	-4.8016210	-0.3206370	6.8290530
B	-2.6073800	-0.5686580	5.4923660
Ge	-1.0220670	2.0036770	9.6354030
Ge	-3.5955630	2.0963470	5.7934020
Ge	1.0151780	1.9599220	5.4853500