Structural trends in ten-vertex endohedral clusters, $M@E_{10}$ and the synthesis of a new member of the family, $[Fe@Sn_{10}]^{3-}$

Tobias Krämer, Jack C. A. Duckworth, Matthew Ingram, Binbin Zhou, John E. McGrady*

and Jose M. Goicoechea*

† Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QR, U.K.

john.mcgrady@chem.ox.ac.uk; jose.goicoechea@chem.ox.ac.uk

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1. Discussion of single crystal X–ray analyses

Single crystal X–ray diffraction data were collected on various crystals of $[K(2,2,2\text{–crypt})]_3[Fe@Sn_{10}]\cdot 4py$ at different temperatures. All of the crystalline samples studied suffer from similar limitations. The crystals are highly air– and moisture–sensitive, small and highly anisotropic in shape (thin black plates). Thus, identifying a good quality specimen, and collecting data without damage to the crystal, was found to be extremely challenging. In general, although the samples were different and problems varied slightly with each data collection, the conclusions discussed below are consistent for all of the crystalline samples studied.All samples were found to exhibit three crystallographically unique $[K(2,2,2\text{–crypt})]^+$ cations alongside an $[Fe@Sn_{10}]^{3-}$ cluster and four pyridine molecules. The cluster anions have an approximately spherical shape and exhibit positional disorder at the cluster site. It is highly likely that such disorder is continuous and not discrete, making its modelling very complex. At best we have been able to model the cluster anion as two separate components. Such disorder is not uncommon in approximately spherical deltahedral clusters and has been observed previously in several other literature–reported species such as $[Ni@Pb_{12}]^{2-}$,[1] $[Ir@Sn_{12}]^{3-}$,[2] $[Ni@Ge_9]^{3-}$,[3] $[Ni@Sn_9Tl]^{3-}$ and $[Pt@Sn_{17}]^{4-}$.[3,4] Positional disorder is not entirely surprising as the cations $[K(2,2,2\text{–crypt})]^+$ leave a void in the lattice that can be occupied by the cluster anion. An approximately spherical cluster has the ability to occupy such a site in multiple orientations, ultimately giving rise to the positional crystallographic disorder observed. Slow cooling of the samples made no apparent difference to the apparent disorder at the cluster site. Attempts to model different clusters on the same site (*i.e.* a solid solution of say $[Fe@Sn_{10}]^{3-}$ and $[Sn_9]^{3-}$) proved unsuccessful. Of all of the data sets collected one of them proved to be optimal in terms of quality (sufficient high angle data, no significant twinning, *etc.*). Full details of data collection are listed below.

A single small black plate (0.30 × 0.12 × 0.05 mm) was mounted on a MitGen loop using Paratone–N oil and quench–cooled using an open flow N_2 cooling device. Single–crystal X–ray diffraction data were collected using an Enraf–Nonius Kappa–CCD diffractometer and a 95 mm CCD area detector with a graphite–monochromated molybdenum K_α source (λ = 0.71073 Å). Data were processed using the DENZO–SMN package, including unit cell parameter refinement and inter–frame scaling (which was carried out using SCALEPACK within DENZO–SMN).[5] Structures were subsequently solved using direct methods, and refined on F^2 using the SHELXL 97–2 package.[6] An initial refinement of the data gives a suitable solution revealing the full contents of the unit cell: $[K(2,2,2\text{–crypt})]_3[Fe@Sn_{10}]\cdot 4py$. The structure refines with relatively high residuals (R1 = 9.00%, wR2 = 24.52% for $I \geq 2\sigma(I)$; R1 = 9.83% and R2 = 25.39% for all data; GoF = 1.027). A close inspection of residual electron density shows a significant amount of positive electron density close to the cluster anion (REM highest difference peak 5.908 $e^-/Å^3$, deepest hole –3.147 $e^-/Å^3$) which is unaccounted for with this model. This and the relatively high values of the weighted residual parameters strongly suggest that there is some positional disorder and/or an unresolved absorption issue. Variations to the absorption correction methodology do not resolve this problem. Despite the possibility of disorder the cluster shows reasonable thermal ellipsoids (Figure S1) for the cluster atoms and it is clear that the geometry adopted by the cluster anion is pseudo–C_{2v} (C_s) not bicapped square antiprismatic (D_{4d}) or pentagonal prismatic (D_{5h}) like previously reported cluster anions $[Ni@Pb_{10}]^{2-}$ (and $[Pb_{10}]^{2-}$) or $[M@Ge_{10}]^{3-}$ (M = Fe, Co), respectively.[2, 8–9]

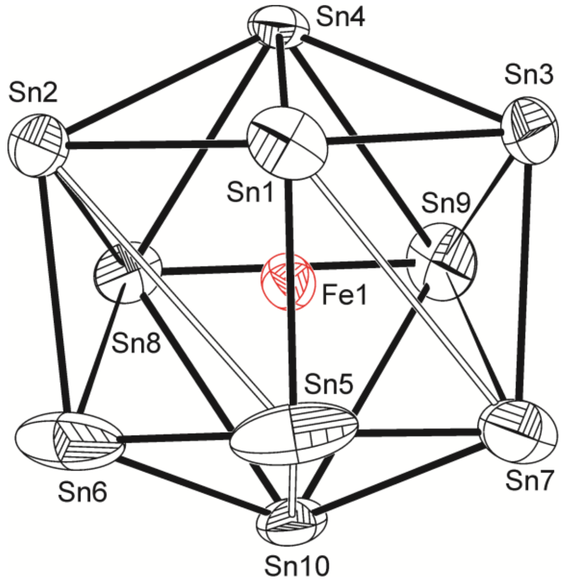

Figure S1. Thermal ellipsoid plot of the $[Fe@Sn_{10}]^{3-}$ present in **1** (without modeling crystallographic disorder at the cluster site). Anisotropic displacement ellipsoids are pictured at the 30% probability level.

The bond metric data within this cluster is close to what might be expected for related Zintl ions (see Table S2) below, however on account of the positional disorder present at the cluster site, interatomic distances and angles cannot be taken as physically meaningful. Fe–Sn bond distances vary between 2.578(3) and 2.808(3) Å. Similarly Sn–Sn bond distances vary between 2.703(5) and 3.2817(18) Å (4.064(3) Å if the open bonds in Figure S3 are considered). There are clearly two bonds which are shorter than the sum of the single bond covalent radii (Sn5–Sn6: 2.703(5) Å and Sn5–Sn7: 2.743(4) Å), with a third very close in magnitude (Sn1–Sn5: 2.816(2) Å), all of which involve the atomic position Sn5.[10]

Table S2. Interatomic distances within the $[Fe@Sn_{10}]^{3-}$ cluster anion (without modelling positional disorder). Numbers in italics represent long Sn–Sn contacts pictured as open bonds in Figure S3).

bond	distance	bond	distance
Fe1–Sn1	2.578(3)	Sn2–Sn6	2.877(2)
Fe1–Sn2	2.808(3)	Sn2–Sn8	3.081 (2)
Fe1–Sn3	2.799(3)	Sn3–Sn4	2.964(2)
Fe1–Sn4	2.622(3)	Sn3–Sn7	2.915(2)

Fe1–Sn5	2.620(3)	Sn3–Sn9	3.080(2)
Fe1–Sn6	2.671(3)	Sn4–Sn8	3.061(2)
Fe1–Sn7	2.696(3)	Sn4–Sn9	3.061(2)
Fe1–Sn8	2.646(3)	Sn5–Sn6	2.703(5)
Fe1–Sn9	2.651(3)	Sn5–Sn7	2.743(4)
Fe1–Sn10	2.648(3)	*Sn5–Sn10*	*3.539(2)*
Sn1–Sn2	2.921(2)	Sn6–Sn8	3.197(2)
Sn1–Sn3	2.908(2)	Sn6–Sn10	2.918(3)
Sn1–Sn4	3.282(2)	Sn7–Sn9	3.222(3)
Sn1–Sn5	2.816(2)	Sn7–Sn10	2.936(2)
Sn1–Sn7	*3.964(3)*	Sn8–Sn9	3.039(2)
Sn2–Sn4	2.961(2)	Sn8–Sn10	3.016(2)
Sn2–Sn5	*4.064(3)*	Sn9–Sn10	3.048(2)

The refinement parameters for this structure improve significantly if a second component is modeled on the cluster anion site. The occupancies of both components were freely refined with the occupation factor of the second component tied to that of the first. The major component refined at 60% occupancy. In order to obtain a physically meaningful refinement it was necessary to refine the second component of the $[Fe@Sn_{10}]^{3-}$ anion by relating all bond metric values to those of the major component employing a similarity restraint (SAME). Ultimately this refinement gives rise to a more suitable structure solution with reasonable residual values (R1 = 5.69%, wR2 = 15.22% for $I \geq 2\sigma(I)$; R1 = 6.48% and R2 = 15.85% for all data; GoF = 1.020). It is important to note, however, that with this refinement the cluster anions still display several unrealistically short Sn–Sn bond distances (Sn–Sn distances vary between 2.585(6) and 3.175(5) Å for the major component). The shortest of these all involve atomic position Sn5 (Sn5–Sn7: 2.585(6) Å; Sn1–Sn5: 2.696(5) Å and Sn5–Sn6: 2.716(4) Å). These distances are even shorter for the minor component. We maintain that in all likelihood this is due to continuous positional disorder of the cluster moiety and the poor suitability of modelling such disorder with a simple two component system.

A final refinement restraining all short Sn–Sn distances to be at least as long as the sum of the covalent single bond radii (2.80 Å) was carried out (R1 = 7.31%, wR2 = 19.93% for $I \geq 2\sigma(I)$; R1 = 8.11% and R2 = 20.67% for all data; GoF = 1.015). The final occupancy of the major component refines to 69%. Due to the inherent disorder at the cluster site (and considering that several Sn–Sn distances had to be fixed in order for them to conform with previously reported values), bond metric data in the cluster anion should not be taken as physically meaningful. However, despite the quality of the data collected and the positional disorder at the cluster site, we have full confidence that three statements can be made about the cluster anion. Firstly, the crystalline phase clearly contains a ten atom tin cluster with an interstitial iron atom (this is corroborated by electrospray mass–

spectrometry). Secondly, the charge associated with the anion is 3– as evidence by the three sequestered potassium cations in $[K(2,2,2\text{–crypt})]^+$. Finally, and this is central to the thesis of this manuscript, it appears that the cluster anion is not bicapped square antiprismatic (D_{4d}) or pentagonal prismatic (D_{5h}) as other previously reported isoelectronic cluster anions.

2. EPR spectroscopy

The room temperature EPR spectrum of a solid sample of **1** reveals a weak and broad resonance centered at g = 2.0229. This resonance sharpens dramatically upon cooling to 15 K and the g value shifts to 2.0297 (Figure S2). These spectra confirm the paramagnetic character of the cluster anion. Similar chemical shifts and broadened resonances have previously been observed for other paramagnetic Zintl ions such as $[Ge_8Fe(CO)_3]^{3-}$ and $[Pb_9]^{3-}$.[11,12] In the case of the former, we observed a similar pronounced temperature dependence of the cluster anion resonance which we attributed to spin-orbit coupling with the atoms of the cluster cage and/or fast relaxation effects.

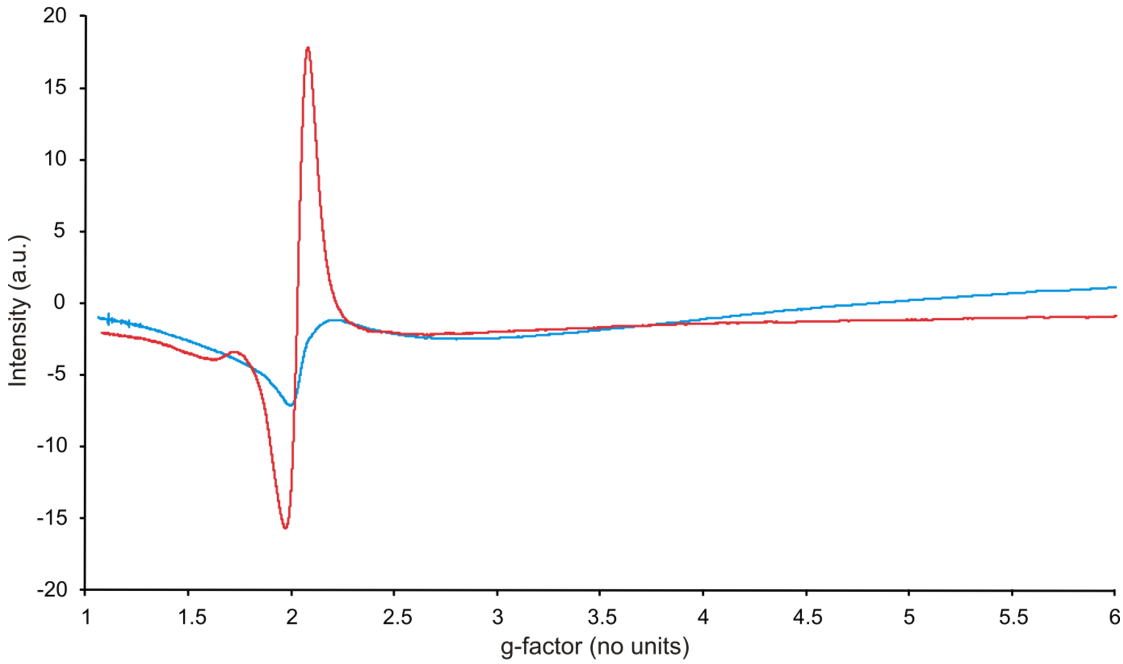

Figure S2. X-band (9.3896 GHz) CW EPR spectrum of a solid sample of **1** recorded at 296 K (blue) and at 15 K (red).

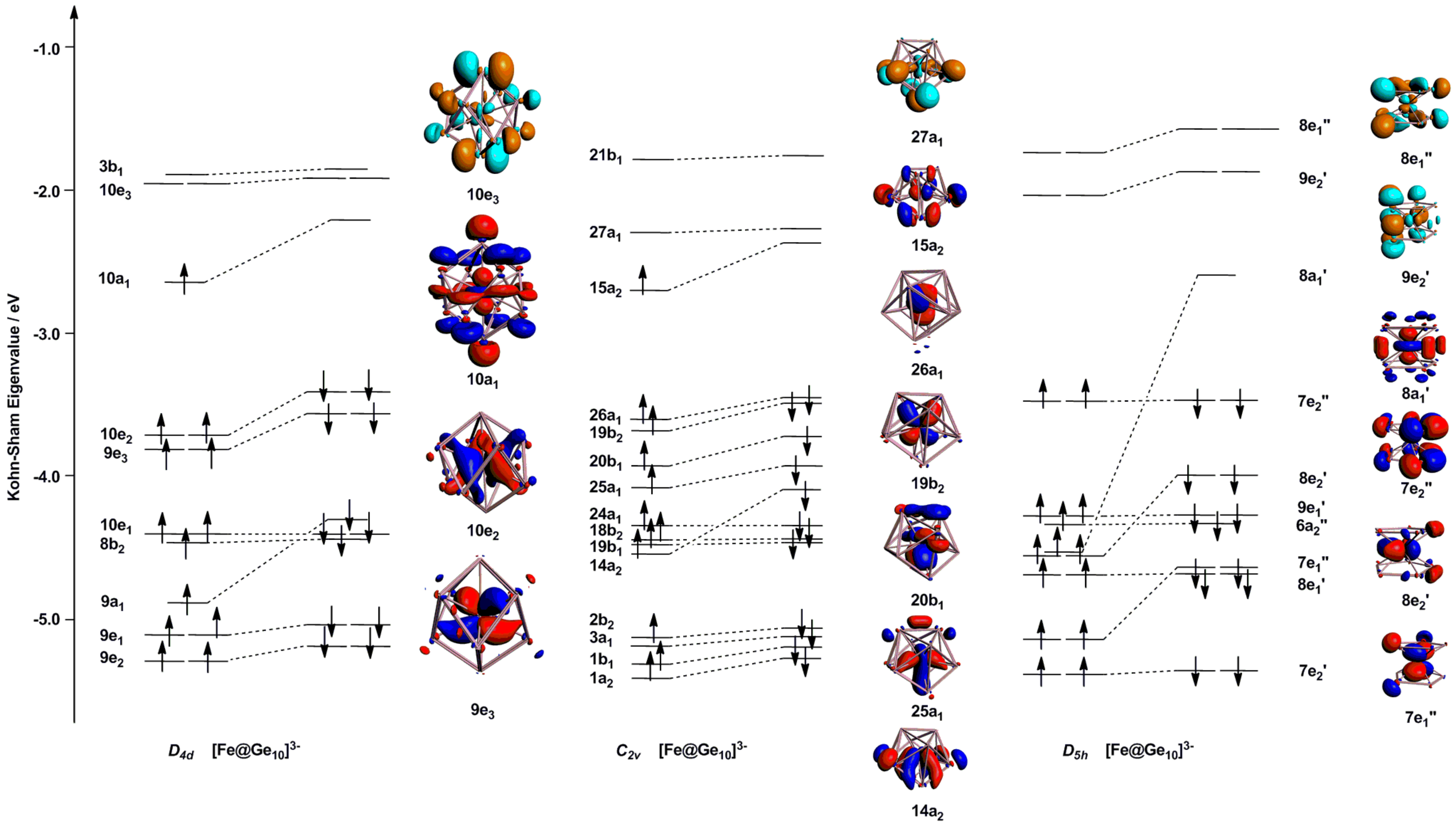

Figure S3. Kohn-Sham eigenvalue diagram (spin-α and spin-β) for the D_{4d}, C_{2v} and D_{5h}–symmetric isomers of $[Fe@Ge_{10}]^{3-}$.

Table S1 Optimised structural parameters for stationary points on the potential energy surface of $[Ni@Pb_{10}]^{2-}$

	D$_{4d}$		*C*$_{3v}$		*C*$_{2v}$		*D*$_{5h}$	
	Ni-Pb(1)	3.40	Ni-Pb(1)	2.66	Ni-Pb(1)	2.76	Ni-Pb(1)	3.01
	Ni-Pb(2)	2.77	Ni-Pb(2)	3.00	Ni-Pb(2)	3.05		
			Ni-Pb(3)	2.94	Ni-Pb(3)	2.86		
			Ni-Pb(4)	2.86	Ni-Pb(4)	2.84		
	Pb(1)-Pb(2)	3.19	Pb(1)-Pb(2)	3.20	Pb(1)-Pb(1)	3.49	Pb(1)-Pb(1)	3.02
	Pb(2)-Pb(2)	3.44	Pb(2)-Pb(2)	4.84	Pb(2)-Pb(2)	3.20	Pb(1)-Pb(1′)	3.15
	Pb(2)-Pb(2′)	3.26	Pb(2)-Pb(3)	3.13	Pb(4)-Pb(4)	3.22		
			Pb(2)-Pb(4)	3.37	Pb(1)-Pb(2)	3.09		
			Pb(3)-Pb(4)	3.25	Pb(1)-Pb(3)	3.42		
			Pb(4)-Pb(4)	3.27	Pb(2)-Pb(4)	3.32		
					Pb(2)-Pb(3)	3.17		
					Pb(1)-Pb(4)	3.29		
2S+1	1		3		1		1	
Energy/ eV	0.0		0.75		0.53		2.09	

Table S2 Optimised structural parameters for stationary points on the potential energy surface of $[Zn@In_{10}]^{8-}$

	D$_{4d}$		*C*$_{3v}$	
	Zn/X-In(1)	2.87	Zn/X-In(1)	2.87
	Zn/X-In(2)	2.87	Zn/X-In(2)	2.85
			Zn/X-In(3)	2.87
			Zn/X-In(4)	2.88
	In(1)-In(2)	3.08	In(1)- In(2)	3.08
	In(2)-In(2)	3.67	In(2)- In(2)	4.49
	In(2)-In(2′)	3.15	In(2)- In(3)	3.07
			In(2)- In(4)	3.45
			In(3)- In(4)	3.21
			In(4)- In(4)	3.26
2S+1		1		1
Energy/ eV		0.0		+0.01

Table S3 Optimised structural parameters for stationary points on the potential energy surface of $[Fe@Ge_{10}]^{3-}$

	D_{4d}		C_{3v}		C_{2v}		D_{5h}	
	Fe-Ge(1)	2.55	Fe-Ge(1)	2.43	Fe-Ge(1)	2.42	Fe-Ge(1)	2.58
	Fe-Ge(2)	2.44	Fe-Ge(2)	2.48	Fe-Ge(2)	2.51		
			Fe-Ge(3)	2.47	Fe-Ge(3)	2.45		
			Fe-Ge(4)	2.44	Fe-Ge(4)	2.42		
	Ge(1)-Ge(2)	2.68	Ge(1)-Ge(2)	2.60	Ge(1)-Ge(1)	2.72	Ge(1)-Ge(1)	2.60
	Ge(2)-Ge(2)	3.12	Ge(2)-Ge(2)	3.85	Ge(2)-Ge(2)	2.68	Ge(1)-Ge(1′)	2.65
	Ge(2)-Ge(2′)	2.67	Ge(2)-Ge(3)	2.65	Ge(3)-Ge(4)	2.76		
			Ge(2)-Ge(4)	3.03	Ge(4)-Ge(4)	2.71		
			Ge(3)-Ge(4)	2.78	Ge(1)-Ge(2)	2.57		
			Ge(4)-Ge(4)	2.72	Ge(1)-Ge(3)	3.17		
					Ge(2)-Ge(3)	2.71		
					Ge(2)-Ge(4)	2.91		
2S+1	2		2		2		2	
$<S^2>$	0.77		0.76		0.77		0.84	
$\rho(Fe)$	0.65		0.36		0.53		1.45	
$\rho(Ge_{10})$	0.35		0.64		0.47		-0.45	
Energy/ eV	+0.37		0.35		+0.26		0.0	

Table S4 Optimised structural parameters for stationary points on the potential energy surface of $[Fe@Sn_{10}]^{3-}$

	D_{4d}		C_{3v}		C_{2v}		D_{5h}	
	Fe-Sn(1)	3.13	Fe-Sn(1)	2.59	Fe-Sn(1)	2.65	Fe-Sn(1)	2.88
	Fe-Sn(2)	2.67	Fe-Sn(2)	2.86	Fe-Sn(2)	2.90		
			Fe-Sn(3)	2.79	Fe-Sn(3)	2.70		
			Fe-Sn(4)	2.69	Fe-Sn(4)	2.68		
	Sn(1)-Sn(2)	3.03	Sn(1)-Sn(2)	2.98	Sn(1)-Sn(2)	3.08	Sn(1)-Sn(1)	2.89
	Sn(2)-Sn(2)	3.35	Sn(2)-Sn(2)	4.53	Sn(2)-Sn(2)	3.02	Sn(1)-Sn(1′)	2.98
	Sn(2)-Sn(2′)	3.06	Sn(2)-Sn(3)	2.98	Sn(3)-Sn(4)	3.12		
			Sn(2)-Sn(4)	3.27	Sn(4)-Sn(4)	3.09		
			Sn(3)-Sn(4)	3.12	Sn(1)-Sn(2)	2.93		
			Sn(4)-Sn(4)	3.12	Sn(1)-Sn(3)	3.38		
					Sn(2)-Sn(3)	3.06		
					Sn(3)-Sn(4)	3.12		
2S+1	2		2		2		2	
$\langle S^2 \rangle$	0.80		1.00		0.94		1.09	
$\rho(Fe)$	1.16		1.08		1.22		1.96	
$\rho(Sn_{10})$	-0.16		-0.08		-0.22		-0.96	
Energy/ eV	+0.03		+0.15		+0.03		+0.32	

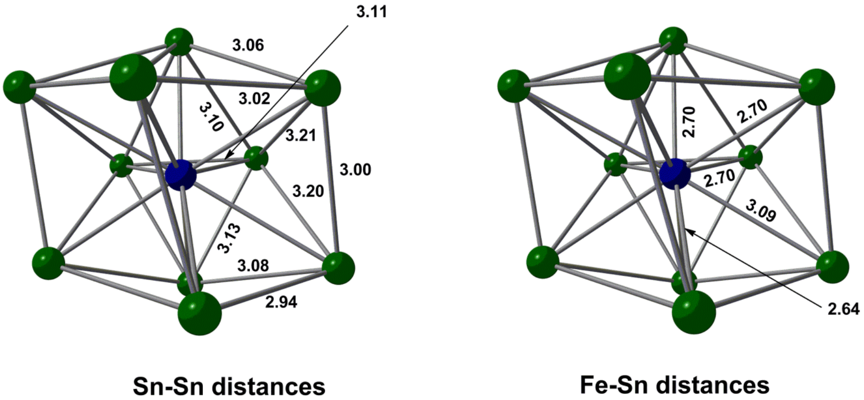

Figure S4. Optimised structural parameters of the C_2-symmetric global minimum of $[Fe@Sn_{10}]^{3-}$.

Table S5. Comparison of optimised structures of $[Zn@In_{10}]^{8-}$ and $[Fe@Sn_{10}]^{3-}$ with their empty counterparts (see Figure 3 for labelling).

	$[Zn@In_{10}]^{8-}$	$[In_{10}]^{10-}$	$[In_{10}]^{12-}$	$[In_{10}]^{14-}$		$[Fe@Sn_{10}]^{3-}$	$[Sn_{10}]^{0}$	$[Sn_{10}]^{2-}$	$[Sn_{10}]^{4-}$
Zn/X-In(1)	2.83	2.80	3.25	3.60	Fe/X-Sn(1)	3.13	2.72	3.18	3.42
Zn/X-In(2)	2.78	2.75	2.64	2.61	Fe/X-Sn(2)	2.67	2.72	2.60	2.57
In(1)-In(2)	3.01	2.96	3.08	3.23	Sn(1)-Sn(2)	3.04	2.91	3.01	3.11
In(2)-In(2)	3.56	3.51	3.33	3.21	Sn(2)-Sn(2)	3.35	3.48	3.24	3.16
In(2)-In(2′)	3.05	3.03	3.06	3.13	Sn(2)-Sn(2′)	3.06	2.99	3.01	3.05

Table S2. Cartesian coordinates of all optimized structures (ADF 2010.02)[1]

1. Germanium clusters, Total Valence Electron Count 51 (*S* = 1/2)

1.1. Pentagonal Prismatic (D_{5h})

1.1.1. $[Fe@Ge_{10}]^{3-}$ / $^2A_1'$ / E = –2.14762631 au / $\langle S^2 \rangle$ = 0.83852

Fe	0.000000000	0.000000000	0.000000000
Ge	1.757545000	-1.276931000	1.323962000
Ge	1.757545000	1.276931000	1.323962000
Ge	-0.671323000	2.066118000	1.323962000
Ge	-2.172445000	0.000000000	1.323962000
Ge	-0.671323000	-2.066118000	1.323962000
Ge	1.757545000	-1.276931000	-1.323962000
Ge	1.757545000	1.276931000	-1.323962000
Ge	-0.671323000	2.066118000	-1.323962000
Ge	-2.172445000	0.000000000	-1.323962000
Ge	-0.671323000	-2.066118000	-1.323962000

1.1.2. $[Co@Ge_{10}]^{2-}$ / $^2E_2''$ / E = –2.00032329 au / $\langle S^2 \rangle$ = 2.25184

Co	0.000000000	0.000000000	0.000000000
Ge	0.668042000	-2.056021000	-1.299651000
Ge	-1.748956000	-1.270691000	-1.299651000
Ge	-1.748956000	1.270691000	-1.299651000
Ge	0.668042000	2.056021000	-1.299651000
Ge	2.161829000	0.000000000	-1.299651000
Ge	0.668042000	-2.056021000	1.299651000
Ge	-1.748956000	-1.270691000	1.299651000
Ge	-1.748956000	1.270691000	1.299651000
Ge	0.668042000	2.056021000	1.299651000
Ge	2.161829000	0.000000000	1.299651000

1.1.3. $[Ni@Ge_{10}]^{1-}$ / $^2E_2''$ / E = –1.77772348 au / $\langle S^2 \rangle$ = 2.25103

Ni	0.000000000	0.000000000	0.000000000
Ge	0.671459000	-2.066539000	-1.301634000
Ge	-1.757903000	-1.277191000	-1.301634000
Ge	-1.757903000	1.277191000	-1.301634000
Ge	0.671459000	2.066539000	-1.301634000
Ge	2.172888000	0.000000000	-1.301634000
Ge	0.671459000	-2.066539000	1.301634000
Ge	-1.757903000	-1.277191000	1.301634000
Ge	-1.757903000	1.277191000	1.301634000
Ge	0.671459000	2.066539000	1.301634000
Ge	2.172888000	0.000000000	1.301634000

1.1.4. $[Cu@Ge_{10}]^{0}$ / $^2E_2''$ / E = –1.52400581 au / $\langle S^2 \rangle$ = 2.25079

Cu	0.000000000	0.000000000	0.000000000
Ge	0.678768000	-2.089032000	-1.308864000
Ge	-1.777037000	-1.291093000	-1.308864000
Ge	-1.777037000	1.291093000	-1.308864000
Ge	0.678768000	2.089032000	-1.308864000

Ge	2.196539000	0.000000000	-1.308864000
Ge	0.678768000	-2.089032000	1.308864000
Ge	-1.777037000	-1.291093000	1.308864000
Ge	-1.777037000	1.291093000	1.308864000
Ge	0.678768000	2.089032000	1.308864000
Ge	2.196539000	0.000000000	1.308864000

1.1.5. $[Zn@Ge_{10}]^{1+}$ / $^{2}E_{2}''$ / E = –1.23567586 au / $\langle S^2\rangle$ = 2.25080

Zn	0.000000000	0.000000000	0.000000000
Ge	0.690249000	-2.124367000	-1.323063000
Ge	-1.807095000	-1.312931000	-1.323063000
Ge	-1.807095000	1.312931000	-1.323063000
Ge	0.690249000	2.124367000	-1.323063000
Ge	2.233692000	0.000000000	-1.323063000
Ge	0.690249000	-2.124367000	1.323063000
Ge	-1.807095000	-1.312931000	1.323063000
Ge	-1.807095000	1.312931000	1.323063000
Ge	0.690249000	2.124367000	1.323063000
Ge	2.233692000	0.000000000	1.323063000

1.2. Bicapped Square Antiprismatic (D_{4d})

1.2.1. $[Fe@Ge_{10}]^{3-}$/ $^{2}A_{1}$ / E = –2.13433647 au / $\langle S^2\rangle$ = 0.76892

Fe	0.000000000	0.000000000	0.000000000
Ge	0.000000000	0.000000000	-2.550192000
Ge	0.000000000	0.000000000	2.550192000
Ge	0.844192000	2.038059000	-1.034157000
Ge	2.038059000	-0.844192000	-1.034157000
Ge	-2.038059000	0.844192000	-1.034157000
Ge	-0.844192000	-2.038059000	-1.034157000
Ge	2.038059000	0.844192000	1.034157000
Ge	-0.844192000	2.038059000	1.034157000
Ge	0.844192000	-2.038059000	1.034157000
Ge	-2.038059000	-0.844192000	1.034157000

1.2.2. $[Co@Ge_{10}]^{2-}$ / $^{2}A_{1}$ / E = –2.02266329 au / $\langle S^2\rangle$ = 0.75731

Co	0.000000000	0.000000000	0.000000000
Ge	0.833973000	-2.013389000	1.050117000
Ge	2.013389000	0.833973000	1.050117000
Ge	-0.833973000	2.013389000	1.050117000
Ge	-2.013389000	-0.833973000	1.050117000
Ge	0.000000000	0.000000000	2.601081000
Ge	2.013389000	-0.833973000	-1.050117000
Ge	0.833973000	2.013389000	-1.050117000
Ge	-2.013389000	0.833973000	-1.050117000
Ge	-0.833973000	-2.013389000	-1.050117000
Ge	0.000000000	0.000000000	-2.601081000

1.2.3. $[Ni@Ge_{10}]^{1-}$ / $^{2}A_{1}$ / E = –1.80866722 au / $\langle S^2\rangle$ = 0.75231

Ni	0.000000000	0.000000000	0.000000000
Ge	0.840255000	-2.028554000	1.055226000
Ge	2.028554000	0.840255000	1.055226000
Ge	-0.840255000	2.028554000	1.055226000

Ge	-2.028554000	-0.840255000	1.055226000
Ge	0.000000000	0.000000000	2.581676000
Ge	2.028554000	-0.840255000	-1.055226000
Ge	0.840255000	2.028554000	-1.055226000
Ge	-2.028554000	0.840255000	-1.055226000
Ge	-0.840255000	-2.028554000	-1.055226000
Ge	0.000000000	0.000000000	-2.581676000

1.2.4. $[Cu@Ge_{10}]^{0}$ / $^{2}A_{1}$ / E = –1.56220709 au / $\langle S^{2}\rangle$ = 0.75236

Cu	0.000000000	0.000000000	0.000000000
Ge	0.850182000	-2.052520000	1.071655000
Ge	2.052520000	0.850182000	1.071655000
Ge	-0.850182000	2.052520000	1.071655000
Ge	-2.052520000	-0.850182000	1.071655000
Ge	0.000000000	0.000000000	2.592118000
Ge	2.052520000	-0.850182000	-1.071655000
Ge	0.850182000	2.052520000	-1.071655000
Ge	-2.052520000	0.850182000	-1.071655000
Ge	-0.850182000	-2.052520000	-1.071655000
Ge	0.000000000	0.000000000	-2.592118000

1.2.5. $[Zn@Ge_{10}]^{1+}$ / $^{2}A_{1}$ / E = –1.27743858 au / $\langle S^{2}\rangle$ = 0.75286

Zn	0.000000000	0.000000000	0.000000000
Ge	0.864007000	-2.085898000	1.097066000
Ge	2.085898000	0.864007000	1.097066000
Ge	-0.864007000	2.085898000	1.097066000
Ge	-2.085898000	-0.864007000	1.097066000
Ge	0.000000000	0.000000000	2.617985000
Ge	2.085898000	-0.864007000	-1.097066000
Ge	0.864007000	2.085898000	-1.097066000
Ge	-2.085898000	0.864007000	-1.097066000
Ge	-0.864007000	-2.085898000	-1.097066000
Ge	0.000000000	0.000000000	-2.617985000

1.3. Tetracapped Trigonal Prismatic (C_{3v})

1.3.1. $[Fe@Ge_{10}]^{3-}$ / $^{2}E_{1}$ / E = –2.13462423 au / $\langle S^{2}\rangle$ = 0.76051

Fe	0.000000000	0.000000000	-0.026911000
Ge	1.112245000	-1.926464000	-1.113641000
Ge	0.000000000	0.000000000	-2.453766000
Ge	2.464222000	0.000000000	0.093305000
Ge	1.112245000	1.926464000	-1.113641000
Ge	0.784321000	-1.358483000	1.841255000
Ge	-2.224489000	0.000000000	-1.113641000
Ge	-1.568641000	0.000000000	1.841255000
Ge	0.784321000	1.358483000	1.841255000
Ge	-1.232111000	-2.134079000	0.093305000
Ge	-1.232111000	2.134079000	0.093305000

1.3.2. $[Co@Ge_{10}]^{2-}$ / $^{2}E_{1}$ / E = –2.01831572 au / $\langle S^{2}\rangle$ = 0.75225

Co	0.000000000	0.000000000	-0.045644000
Ge	1.572870000	0.000000000	1.835412000
Ge	-0.786435000	-1.362145000	1.835412000

Ge	2.232478000	0.000000000	-1.098932000
Ge	0.000000000	0.000000000	-2.444657000
Ge	-2.457056000	0.000000000	0.094307000
Ge	1.228528000	2.127873000	0.094307000
Ge	-1.116239000	-1.933383000	-1.098932000
Ge	1.228528000	-2.127873000	0.094307000
Ge	-0.786435000	1.362145000	1.835412000
Ge	-1.116239000	1.933383000	-1.098932000

1.3.3. $[Ni@Ge_{10}]^{1-}$ / $^2E_1$/ E = –1.80056005 au / $\langle S^2 \rangle$ = 0.75205

Ni	0.000000000	0.000000000	-0.071532000
Ge	1.583255000	0.000000000	1.835421000
Ge	-0.791627000	-1.371139000	1.835421000
Ge	2.249881000	0.000000000	-1.087964000
Ge	0.000000000	0.000000000	-2.468993000
Ge	-2.467525000	0.000000000	0.096745000
Ge	1.233762000	2.136939000	0.096745000
Ge	-1.124941000	-1.948455000	-1.087964000
Ge	1.233762000	-2.136939000	0.096745000
Ge	-0.791627000	1.371139000	1.835421000
Ge	-1.124941000	1.948455000	-1.087964000

1.3.4. $[Cu@Ge_{10}]^{0}$ / $^2E_1$ / E = –1.55015658 au / $\langle S^2 \rangle$ = 0.75263

Cu	0.000000000	0.000000000	-0.084031000
Ge	1.602558000	0.000000000	1.852842000
Ge	-0.801279000	-1.387856000	1.852842000
Ge	2.281930000	0.000000000	-1.085817000
Ge	0.000000000	0.000000000	-2.508824000
Ge	-2.490134000	0.000000000	0.101892000
Ge	1.245067000	2.156519000	0.101892000
Ge	-1.140965000	-1.976209000	-1.085817000
Ge	1.245067000	-2.156519000	0.101892000
Ge	-0.801279000	1.387856000	1.852842000
Ge	-1.140965000	1.976209000	-1.085817000

1.3.5. $[Zn@Ge_{10}]^{1+}$/ $^2E_1$ / E = –1.26228333 au / $\langle S^2 \rangle$ = 0.75307

Zn	0.000000000	0.000000000	-0.083749000
Ge	1.633612000	0.000000000	1.873623000
Ge	-0.816806000	-1.414750000	1.873623000
Ge	2.324170000	0.000000000	-1.092929000
Ge	0.000000000	0.000000000	-2.568225000
Ge	-2.532539000	0.000000000	0.109578000
Ge	1.266269000	2.193243000	0.109578000
Ge	-1.162085000	-2.012790000	-1.092929000
Ge	1.266269000	-2.193243000	0.109578000
Ge	-0.816806000	1.414750000	1.873623000
Ge	-1.162085000	2.012790000	-1.092929000

1.4. *nido*-Octadecahedron (C_{2v})

1.4.1. $[Fe@Ge_{10}]^{3-}$/ $^2A_2$ / E = –2.13802395 au / $\langle S^2 \rangle$ = 0.76671

Fe	0.000000000	0.000000000	-0.020798000
Ge	-1.360811000	0.000000000	-2.023238000
Ge	1.360811000	0.000000000	-2.023238000

Ge	-1.338525000	-2.066379000	-0.495845000
Ge	1.338525000	-2.066379000	-0.495845000
Ge	-2.205583000	0.000000000	1.034025000
Ge	1.338525000	2.066379000	-0.495845000
Ge	0.000000000	1.354949000	1.984795000
Ge	0.000000000	-1.354949000	1.984795000
Ge	-1.338525000	2.066379000	-0.495845000
Ge	2.205583000	0.000000000	1.034025000

1.4.2. $[Co@Ge_{10}]^{2-}$ / $^{2}A_2$ / E = –2.02289772 au / $\langle S^2 \rangle$ = 0.75483

Co	0.000000000	0.000000000	0.051507000
Ge	-2.200557000	0.000000000	-1.012384000
Ge	-1.376392000	0.000000000	2.020058000
Ge	1.334195000	2.067345000	0.478759000
Ge	0.000000000	1.349269000	-1.985278000
Ge	-1.334195000	2.067345000	0.478759000
Ge	-1.334195000	-2.067345000	0.478759000
Ge	1.376392000	0.000000000	2.020058000
Ge	2.200557000	0.000000000	-1.012384000
Ge	0.000000000	-1.349269000	-1.985278000
Ge	1.334195000	-2.067345000	0.478759000

1.4.3. $[Ni@Ge_{10}]^{1-}$ / $^{2}A_2$ / E = –1.80617257 au / $\langle S^2 \rangle$ = 0.75250

Ni	0.000000000	0.000000000	0.083464000
Ge	-2.208297000	0.000000000	-1.002137000
Ge	-1.409009000	0.000000000	2.028766000
Ge	1.338661000	2.076911000	0.468262000
Ge	0.000000000	1.349849000	-1.995561000
Ge	-1.338661000	2.076911000	0.468262000
Ge	-1.338661000	-2.076911000	0.468262000
Ge	1.409009000	0.000000000	2.028766000
Ge	2.208297000	0.000000000	-1.002137000
Ge	0.000000000	-1.349849000	-1.995561000
Ge	1.338661000	-2.076911000	0.468262000

1.4.4. $[Cu@Ge_{10}]^{0}$ / $^{2}A_2$ / E = –1.55729743 au / $\langle S^2 \rangle$ = 0.75282

Cu	0.000000000	0.000000000	0.108951000
Ge	-2.233299000	0.000000000	-0.991115000
Ge	-1.470758000	0.000000000	2.042547000
Ge	1.356587000	2.101254000	0.460386000
Ge	0.000000000	1.359676000	-2.017537000
Ge	-1.356587000	2.101254000	0.460386000
Ge	-1.356587000	-2.101254000	0.460386000
Ge	1.470758000	0.000000000	2.042547000
Ge	2.233299000	0.000000000	-0.991115000
Ge	0.000000000	-1.359676000	-2.017537000
Ge	1.356587000	-2.101254000	0.460386000

1.4.5. $[Zn@Ge_{10}]^{1+}$ / $^{2}A_2$ / E = –1.27131664 au / $\langle S^2 \rangle$ = 0.75327

Zn	0.000000000	0.000000000	0.152460000
Ge	-2.273114000	0.000000000	-0.983285000
Ge	-1.601787000	0.000000000	2.052473000
Ge	1.388517000	2.135945000	0.452653000
Ge	0.000000000	1.374753000	-2.039227000

Ge	-1.388517000	2.135945000	0.452653000
Ge	-1.388517000	-2.135945000	0.452653000
Ge	1.601787000	0.000000000	2.052473000
Ge	2.273114000	0.000000000	-0.983285000
Ge	0.000000000	-1.374753000	-2.039227000
Ge	1.388517000	-2.135945000	0.452653000

2. Germanium clusters, Total Valence Electron Count 52 (S = 0)

2.1. Pentagonal Prismatic (D_{5h})

2.1.1. $[Fe@Ge_{10}]^{4-}$ / $^1A_1'$ / E = –2.23757988 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	0.000000000
Ge	0.667022000	-2.052883000	-1.323582000
Ge	-1.746287000	-1.268752000	-1.323582000
Ge	-1.746287000	1.268752000	-1.323582000
Ge	0.667022000	2.052883000	-1.323582000
Ge	2.158529000	0.000000000	-1.323582000
Ge	0.667022000	-2.052883000	1.323582000
Ge	-1.746287000	-1.268752000	1.323582000
Ge	-1.746287000	1.268752000	1.323582000
Ge	0.667022000	2.052883000	1.323582000
Ge	2.158529000	0.000000000	1.323582000

2.1.2. $[Co@Ge_{10}]^{3-}$ / $^1A_1'$ / E = –2.12850223 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	0.000000000
Ge	0.666910000	-2.052539000	-1.321617000
Ge	-1.745994000	-1.268539000	-1.321617000
Ge	-1.745994000	1.268539000	-1.321617000
Ge	0.666910000	2.052539000	-1.321617000
Ge	2.158167000	0.000000000	-1.321617000
Ge	0.666910000	-2.052539000	1.321617000
Ge	-1.745994000	-1.268539000	1.321617000
Ge	-1.745994000	1.268539000	1.321617000
Ge	0.666910000	2.052539000	1.321617000
Ge	2.158167000	0.000000000	1.321617000

2.1.3. $[Ni@Ge_{10}]^{2-}$ / $^1A_1'$ / E = –1.91877535 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	0.000000000
Ge	0.669817000	-2.061485000	-1.324045000
Ge	-1.753604000	-1.274068000	-1.324045000
Ge	-1.753604000	1.274068000	-1.324045000
Ge	0.669817000	2.061485000	-1.324045000
Ge	2.167574000	0.000000000	-1.324045000
Ge	0.669817000	-2.061485000	1.324045000
Ge	-1.753604000	-1.274068000	1.324045000
Ge	-1.753604000	1.274068000	1.324045000
Ge	0.669817000	2.061485000	1.324045000
Ge	2.167574000	0.000000000	1.324045000

2.1.4. $[Cu@Ge_{10}]^{1-}$ / $^1A_1'$ / E = –1.67988256 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	0.000000000
Ge	0.677731000	-2.085841000	-1.332664000
Ge	-1.774322000	-1.289120000	-1.332664000
Ge	-1.774322000	1.289120000	-1.332664000
Ge	0.677731000	2.085841000	-1.332664000
Ge	2.193183000	0.000000000	-1.332664000
Ge	0.677731000	-2.085841000	1.332664000
Ge	-1.774322000	-1.289120000	1.332664000
Ge	-1.774322000	1.289120000	1.332664000
Ge	0.677731000	2.085841000	1.332664000
Ge	2.193183000	0.000000000	1.332664000

2.1.5. $[Zn@Ge_{10}]^{0}$ / $^{1}A_{1}'$ / E = –1.40662320 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	0.000000000
Ge	0.688499000	-2.118983000	-1.349567000
Ge	-1.802515000	-1.309604000	-1.349567000
Ge	-1.802515000	1.309604000	-1.349567000
Ge	0.688499000	2.118983000	-1.349567000
Ge	2.228031000	0.000000000	-1.349567000
Ge	0.688499000	-2.118983000	1.349567000
Ge	-1.802515000	-1.309604000	1.349567000
Ge	-1.802515000	1.309604000	1.349567000
Ge	0.688499000	2.118983000	1.349567000
Ge	2.228031000	0.000000000	1.349567000

2.2. Bicapped Square Antiprismatic (D_{4d})

2.2.1. $[Fe@Ge_{10}]^{4-}$ / $^{1}A_{1}$ / E = –2.21118636 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	0.000000000
Ge	0.857084000	-2.069184000	1.018852000
Ge	2.069184000	0.857084000	1.018852000
Ge	-0.857084000	2.069184000	1.018852000
Ge	-2.069184000	-0.857084000	1.018852000
Ge	0.000000000	0.000000000	2.488894000
Ge	2.069184000	-0.857084000	-1.018852000
Ge	0.857084000	2.069184000	-1.018852000
Ge	-2.069184000	0.857084000	-1.018852000
Ge	-0.857084000	-2.069184000	-1.018852000
Ge	0.000000000	0.000000000	-2.488894000

2.2.2. $[Co@Ge_{10}]^{3-}$ / $^{1}A_{1}$ / E = –2.11853961 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	0.000000000
Ge	0.834698000	-2.015140000	1.052577000
Ge	2.015140000	0.834698000	1.052577000
Ge	-0.834698000	2.015140000	1.052577000
Ge	-2.015140000	-0.834698000	1.052577000
Ge	0.000000000	0.000000000	2.616991000
Ge	2.015140000	-0.834698000	-1.052577000
Ge	0.834698000	2.015140000	-1.052577000
Ge	-2.015140000	0.834698000	-1.052577000
Ge	-0.834698000	-2.015140000	-1.052577000
Ge	0.000000000	0.000000000	-2.616991000

2.2.3. $[Ni@Ge_{10}]^{2-}$ / $^{1}A_{1}$ / E = –1.93180316 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	0.000000000
Ge	0.824309000	-1.990057000	1.082501000
Ge	1.990057000	0.824309000	1.082501000
Ge	-0.824309000	1.990057000	1.082501000
Ge	-1.990057000	-0.824309000	1.082501000
Ge	0.000000000	0.000000000	2.722463000
Ge	1.990057000	-0.824309000	-1.082501000
Ge	0.824309000	1.990057000	-1.082501000
Ge	-1.990057000	0.824309000	-1.082501000
Ge	-0.824309000	-1.990057000	-1.082501000
Ge	0.000000000	0.000000000	-2.722463000

2.2.4. $[Cu@Ge_{10}]^{1-}$ / $^{1}A_1$ / E = –1.71090366 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	0.000000000
Ge	0.830853000	-2.005858000	1.100553000
Ge	2.005858000	0.830853000	1.100553000
Ge	-0.830853000	2.005858000	1.100553000
Ge	-2.005858000	-0.830853000	1.100553000
Ge	0.000000000	0.000000000	2.768811000
Ge	2.005858000	-0.830853000	-1.100553000
Ge	0.830853000	2.005858000	-1.100553000
Ge	-2.005858000	0.830853000	-1.100553000
Ge	-0.830853000	-2.005858000	-1.100553000
Ge	0.000000000	0.000000000	-2.768811000

2.2.5. $[Zn@Ge_{10}]^{0}$ / $^{1}A_1$ / E = –1.44615170 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	0.000000000
Ge	0.846818000	-2.044399000	1.119788000
Ge	2.044399000	0.846818000	1.119788000
Ge	-0.846818000	2.044399000	1.119788000
Ge	-2.044399000	-0.846818000	1.119788000
Ge	0.000000000	0.000000000	2.786998000
Ge	2.044399000	-0.846818000	-1.119788000
Ge	0.846818000	2.044399000	-1.119788000
Ge	-2.044399000	0.846818000	-1.119788000
Ge	-0.846818000	-2.044399000	-1.119788000
Ge	0.000000000	0.000000000	-2.786998000

2.3. Tetracapped Trigonal Prismatic (C_{3v})

2.3.1. $[Fe@Ge_{10}]^{4-}$ / $^{1}A_1$ / E = –2.20352802 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	0.179726000
Ge	1.580822000	0.000000000	2.144025000
Ge	-0.790411000	-1.369032000	2.144025000
Ge	1.666423000	0.000000000	-1.496890000
Ge	0.000000000	0.000000000	-3.519876000
Ge	-2.358376000	0.000000000	0.480826000
Ge	1.179188000	2.042413000	0.480826000
Ge	-0.833212000	-1.443165000	-1.496890000
Ge	1.179188000	-2.042413000	0.480826000
Ge	-0.790411000	1.369032000	2.144025000
Ge	-0.833212000	1.443165000	-1.496890000

2.3.2. $[Co@Ge_{10}]^{3-}$ / $^1A_1$ / E = –2.10201843 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	0.225879000
Ge	1.582192000	0.000000000	2.067201000
Ge	-0.791096000	-1.370218000	2.067201000
Ge	1.725931000	0.000000000	-1.344446000
Ge	0.000000000	0.000000000	-3.342872000
Ge	-2.415789000	0.000000000	0.335280000
Ge	1.207895000	2.092135000	0.335280000
Ge	-0.862965000	-1.494700000	-1.344446000
Ge	1.207895000	-2.092135000	0.335280000
Ge	-0.791096000	1.370218000	2.067201000
Ge	-0.862965000	1.494700000	-1.344446000

2.3.3. $[Ni@Ge_{10}]^{2-}$ / $^1A_1$ / E = –1.90420242 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	0.248867000
Ge	1.582136000	0.000000000	2.059054000
Ge	-0.791068000	-1.370170000	2.059054000
Ge	1.750045000	0.000000000	-1.301680000
Ge	0.000000000	0.000000000	-3.295238000
Ge	-2.464021000	0.000000000	0.278540000
Ge	1.232010000	2.133905000	0.278540000
Ge	-0.875023000	-1.515584000	-1.301680000
Ge	1.232010000	-2.133905000	0.278540000
Ge	-0.791068000	1.370170000	2.059054000
Ge	-0.875023000	1.515584000	-1.301680000

2.3.4. $[Cu@Ge_{10}]^{1-}$ / $^1A_1$ / E = –1.67361419 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	0.265980000
Ge	1.589409000	0.000000000	2.095459000
Ge	-0.794705000	-1.376469000	2.095459000
Ge	1.773029000	0.000000000	-1.309509000
Ge	0.000000000	0.000000000	-3.296485000
Ge	-2.502847000	0.000000000	0.246199000
Ge	1.251424000	2.167529000	0.246199000
Ge	-0.886514000	-1.535488000	-1.309509000
Ge	1.251424000	-2.167529000	0.246199000
Ge	-0.794705000	1.376469000	2.095459000
Ge	-0.886514000	1.535488000	-1.309509000

2.3.5. $[Zn@Ge_{10}]^{0}$ / $^1A_1$ / E = –1.40237905 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	0.285863000
Ge	1.595761000	0.000000000	2.169598000
Ge	-0.797880000	-1.381969000	2.169598000
Ge	1.817194000	0.000000000	-1.329341000
Ge	0.000000000	0.000000000	-3.301491000
Ge	-2.539635000	0.000000000	0.187886000
Ge	1.269818000	2.199389000	0.187886000
Ge	-0.908597000	-1.573736000	-1.329341000
Ge	1.269818000	-2.199389000	0.187886000
Ge	-0.797880000	1.381969000	2.169598000
Ge	-0.908597000	1.573736000	-1.329341000

2.4. *nido*-Octadecahedron (C_{2v})

2.4.1. $[Fe@Ge_{10}]^{4-}$ / $^{1}A_1$ / E = –2.22015820 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	-0.044574000
Ge	-2.436284000	0.000000000	0.817958000
Ge	0.000000000	1.334215000	1.905182000
Ge	1.439007000	2.069949000	-0.397313000
Ge	-1.537441000	0.000000000	-1.911650000
Ge	-1.439007000	2.069949000	-0.397313000
Ge	0.000000000	-1.334215000	1.905182000
Ge	2.436284000	0.000000000	0.817958000
Ge	1.537441000	0.000000000	-1.911650000
Ge	-1.439007000	-2.069949000	-0.397313000
Ge	1.439007000	-2.069949000	-0.397313000

2.4.2. $[Co@Ge_{10}]^{3-}$ / $^{1}A_1$ / E = –2.12217916 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	-0.066210000
Ge	-2.275217000	0.000000000	0.918848000
Ge	0.000000000	1.337114000	1.940253000
Ge	1.387328000	2.096052000	-0.453587000
Ge	-1.523086000	0.000000000	-1.926865000
Ge	-1.387328000	2.096052000	-0.453587000
Ge	0.000000000	-1.337114000	1.940253000
Ge	2.275217000	0.000000000	0.918848000
Ge	1.523086000	0.000000000	-1.926865000
Ge	-1.387328000	-2.096052000	-0.453587000
Ge	1.387328000	-2.096052000	-0.453587000

2.4.3. $[Ni@Ge_{10}]^{2-}$ / $^{1}A_1$ / E = –1.92729371 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	-0.097484000
Ge	-2.238822000	0.000000000	0.926316000
Ge	0.000000000	1.340893000	1.960162000
Ge	1.391500000	2.124052000	-0.462104000
Ge	-1.557320000	0.000000000	-1.924955000
Ge	-1.391500000	2.124052000	-0.462104000
Ge	0.000000000	-1.340893000	1.960162000
Ge	2.238822000	0.000000000	0.926316000
Ge	1.557320000	0.000000000	-1.924955000
Ge	-1.391500000	-2.124052000	-0.462104000
Ge	1.391500000	-2.124052000	-0.462104000

2.4.4. $[Cu@Ge_{10}]^{1-}$ / $^{1}A_1$ / E = –1.70226733 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	-0.185530000
Ge	-2.235964000	0.000000000	0.926318000
Ge	0.000000000	1.348983000	1.965659000
Ge	1.425473000	2.155575000	-0.454204000
Ge	-1.707738000	0.000000000	-1.907698000
Ge	-1.425473000	2.155575000	-0.454204000
Ge	0.000000000	-1.348983000	1.965659000
Ge	2.235964000	0.000000000	0.926318000
Ge	1.707738000	0.000000000	-1.907698000
Ge	-1.425473000	-2.155575000	-0.454204000
Ge	1.425473000	-2.155575000	-0.454204000

2.4.5. $[Zn@Ge_{10}]^0$ / $^1A_1$ / E = –1.44161570 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	-0.462820000
Ge	-2.195508000	0.000000000	0.953698000
Ge	0.000000000	1.368185000	1.936431000
Ge	1.505816000	2.188055000	-0.430100000
Ge	-2.078254000	0.000000000	-1.835804000
Ge	-1.505816000	2.188055000	-0.430100000
Ge	0.000000000	-1.368185000	1.936431000
Ge	2.195508000	0.000000000	0.953698000
Ge	2.078254000	0.000000000	-1.835804000
Ge	-1.505816000	-2.188055000	-0.430100000
Ge	1.505816000	-2.188055000	-0.430100000

3. Tin clusters, Total Valence Electron Count 51 (S = 1/2)

3.1. Pentagonal Prismatic (D_{5h})

3.1.1. $[Fe@Sn_{10}]^{3-}$ / $^2A_1'$ / E = –1.90858789 au / $\langle S^2 \rangle$ = 1.08583

Fe	0.000000000	0.000000000	0.000000000
Sn	2.458866000	0.000000000	-1.489110000
Sn	2.458866000	0.000000000	1.489110000
Sn	0.759831000	2.338520000	1.489110000
Sn	0.759831000	-2.338520000	1.489110000
Sn	0.759831000	2.338520000	-1.489110000
Sn	0.759831000	-2.338520000	-1.489110000
Sn	-1.989264000	1.445285000	1.489110000
Sn	-1.989264000	-1.445285000	1.489110000
Sn	-1.989264000	1.445285000	-1.489110000
Sn	-1.989264000	-1.445285000	-1.489110000

3.1.2. $[Co@Sn_{10}]^{2-}$ / $^2A_1'$ / E = –1.76191801 au / $\langle S^2 \rangle$ = 0.82019

Co	0.000000000	0.000000000	0.000000000
Sn	1.990266000	1.446013000	-1.491652000
Sn	1.990266000	-1.446013000	-1.491652000
Sn	-0.760214000	-2.339698000	-1.491652000
Sn	-2.460104000	0.000000000	-1.491652000
Sn	-0.760214000	2.339698000	-1.491652000
Sn	1.990266000	1.446013000	1.491652000
Sn	1.990266000	-1.446013000	1.491652000
Sn	-0.760214000	-2.339698000	1.491652000
Sn	-2.460104000	0.000000000	1.491652000
Sn	-0.760214000	2.339698000	1.491652000

3.1.3. $[Ni@Sn_{10}]^{1-}$ / $^2E_2''$ / E = –1.54996142 au / $\langle S^2 \rangle$ = 2.25115

Ni	0.000000000	0.000000000	0.000000000
Sn	-1.983988000	1.441452000	1.471557000
Sn	-1.983988000	-1.441452000	1.471557000
Sn	0.757816000	-2.332318000	1.471557000
Sn	2.452344000	0.000000000	1.471557000
Sn	0.757816000	2.332318000	1.471557000
Sn	-1.983988000	1.441452000	-1.471557000
Sn	-1.983988000	-1.441452000	-1.471557000

Sn	0.757816000	-2.332318000	-1.471557000
Sn	2.452344000	0.000000000	-1.471557000
Sn	0.757816000	2.332318000	-1.471557000

3.1.4. $[Cu@Sn_{10}]^{0}$ / $^{2}E_2''$ / E = –1.32272442 au / $\langle S^2 \rangle$ = 2.25077

Cu	0.000000000	0.000000000	0.000000000
Sn	-2.008350000	-1.459152000	-1.481885000
Sn	-2.008350000	1.459152000	-1.481885000
Sn	0.767121000	2.360957000	-1.481885000
Sn	2.482457000	0.000000000	-1.481885000
Sn	0.767121000	-2.360957000	-1.481885000
Sn	-2.008350000	-1.459152000	1.481885000
Sn	-2.008350000	1.459152000	1.481885000
Sn	0.767121000	2.360957000	1.481885000
Sn	2.482457000	0.000000000	1.481885000
Sn	0.767121000	-2.360957000	1.481885000

3.1.5. $[Zn@Sn_{10}]^{1+}$ / $^{2}E_2''$ / E = –1.06470111 au / $\langle S^2 \rangle$ = 2.25078

Zn	0.000000000	0.000000000	0.000000000
Sn	-2.036024000	1.479258000	1.498962000
Sn	-2.036024000	-1.479258000	1.498962000
Sn	0.777692000	-2.393490000	1.498962000
Sn	2.516664000	0.000000000	1.498962000
Sn	0.777692000	2.393490000	1.498962000
Sn	-2.036024000	1.479258000	-1.498962000
Sn	-2.036024000	-1.479258000	-1.498962000
Sn	0.777692000	-2.393490000	-1.498962000
Sn	2.516664000	0.000000000	-1.498962000
Sn	0.777692000	2.393490000	-1.498962000

3.2. Bicapped Square Antiprismatic (D_{4d})

3.2.1. $[Fe@Sn_{10}]^{3-}$ / $^{2}A_1$ / E = –1.92017038 au / $\langle S^2 \rangle$ = 0.80108

Fe	0.000000000	0.000000000	0.000000000
Sn	0.000000000	0.000000000	-3.130311000
Sn	0.000000000	0.000000000	3.130311000
Sn	0.906995000	2.189681000	-1.232418000
Sn	2.189681000	-0.906995000	-1.232418000
Sn	-2.189681000	0.906995000	-1.232418000
Sn	-0.906995000	-2.189681000	-1.232418000
Sn	2.189681000	0.906995000	1.232418000
Sn	-0.906995000	2.189681000	1.232418000
Sn	0.906995000	-2.189681000	1.232418000
Sn	-2.189681000	-0.906995000	1.232418000

3.2.2. $[Co@Sn_{10}]^{2-}$ / $^{2}A_1$ / E = –1.81259056 au / $\langle S^2 \rangle$ = 0.76745

Co	0.000000000	0.000000000	0.000000000
Sn	0.911326000	-2.200135000	1.219505000
Sn	2.200135000	0.911326000	1.219505000
Sn	-0.911326000	2.200135000	1.219505000
Sn	-2.200135000	-0.911326000	1.219505000
Sn	0.000000000	0.000000000	3.085371000
Sn	2.200135000	-0.911326000	-1.219505000
Sn	0.911326000	2.200135000	-1.219505000

Sn	-2.200135000	0.911326000	-1.219505000
Sn	-0.911326000	-2.200135000	-1.219505000
Sn	0.000000000	0.000000000	-3.085371000

3.2.3. $[Ni@Sn_{10}]^{1-}$/ $^{2}A_1$ / E = –1.60942861 au / $\langle S^2 \rangle$ = 0.75286

Ni	0.000000000	0.000000000	0.000000000
Sn	0.922883000	-2.228037000	1.206759000
Sn	2.228037000	0.922883000	1.206759000
Sn	-0.922883000	2.228037000	1.206759000
Sn	-2.228037000	-0.922883000	1.206759000
Sn	0.000000000	0.000000000	3.001520000
Sn	2.228037000	-0.922883000	-1.206759000
Sn	0.922883000	2.228037000	-1.206759000
Sn	-2.228037000	0.922883000	-1.206759000
Sn	-0.922883000	-2.228037000	-1.206759000
Sn	0.000000000	0.000000000	-3.001520000

3.2.4. $[Cu@Sn_{10}]^{0}$/ $^{2}A_1$ / E = –1.38608789 au / $\langle S^2 \rangle$ = 0.75231

Cu	0.000000000	0.000000000	0.000000000
Sn	0.941149000	-2.272135000	1.213541000
Sn	2.272135000	0.941149000	1.213541000
Sn	-0.941149000	2.272135000	1.213541000
Sn	-2.272135000	-0.941149000	1.213541000
Sn	0.000000000	0.000000000	2.961310000
Sn	2.272135000	-0.941149000	-1.213541000
Sn	0.941149000	2.272135000	-1.213541000
Sn	-2.272135000	0.941149000	-1.213541000
Sn	-0.941149000	-2.272135000	-1.213541000
Sn	0.000000000	0.000000000	-2.961310000

3.2.5. $[Zn@Sn_{10}]^{1+}$/ $^{2}A_1$ / E = –1.12700437 au / $\langle S^2 \rangle$ = 0.75276

Zn	0.000000000	0.000000000	0.000000000
Sn	0.957851000	-2.312457000	1.233624000
Sn	2.312457000	0.957851000	1.233624000
Sn	-0.957851000	2.312457000	1.233624000
Sn	-2.312457000	-0.957851000	1.233624000
Sn	0.000000000	0.000000000	2.982197000
Sn	2.312457000	-0.957851000	-1.233624000
Sn	0.957851000	2.312457000	-1.233624000
Sn	-2.312457000	0.957851000	-1.233624000
Sn	-0.957851000	-2.312457000	-1.233624000
Sn	0.000000000	0.000000000	-2.982197000

3.3.Tetracapped Trigonal Prismatic (C_{3v})

3.3.1. $[Fe@Sn_{10}]^{3-}$ / $^{2}E_1$ / E = –1.91465727 au / $\langle S^2 \rangle$ = 1.00395

Fe	0.000000000	0.000000000	-0.016400000
Sn	1.306790000	-2.263427000	-1.176958000
Sn	0.000000000	0.000000000	-2.606869000
Sn	2.793273000	0.000000000	0.061320000
Sn	1.306790000	2.263427000	-1.176958000
Sn	0.899084000	-1.557260000	1.984087000
Sn	-2.613580000	0.000000000	-1.176958000
Sn	-1.798169000	0.000000000	1.984087000

Sn	0.899084000	1.557260000	1.984087000
Sn	-1.396637000	-2.419046000	0.061320000
Sn	-1.396637000	2.419046000	0.061320000

3.3.2. $[Co@Sn_{10}]^{2-}$ / $^2E_1$ / E = –1.80052215 au / $\langle S^2 \rangle$ = 0.76473

Co	0.000000000	0.000000000	-0.082592000
Sn	1.781740000	0.000000000	1.992517000
Sn	-0.890870000	-1.543032000	1.992517000
Sn	2.543786000	0.000000000	-1.196887000
Sn	0.000000000	0.000000000	-2.706566000
Sn	-2.776529000	0.000000000	0.095439000
Sn	1.388265000	2.404545000	0.095439000
Sn	-1.271893000	-2.202983000	-1.196887000
Sn	1.388265000	-2.404545000	0.095439000
Sn	-0.890870000	1.543032000	1.992517000
Sn	-1.271893000	2.202983000	-1.196887000

3.3.3. $[Ni@Sn_{10}]^{1-}$ / $^2E_1$ / E = –1.59776161 au / $\langle S^2 \rangle$ = 0.75206

Ni	0.000000000	0.000000000	-0.094126000
Sn	1.788620000	0.000000000	2.010699000
Sn	-0.894310000	-1.548991000	2.010699000
Sn	2.556433000	0.000000000	-1.202234000
Sn	0.000000000	0.000000000	-2.728041000
Sn	-2.769386000	0.000000000	0.090617000
Sn	1.384693000	2.398359000	0.090617000
Sn	-1.278216000	-2.213936000	-1.202234000
Sn	1.384693000	-2.398359000	0.090617000
Sn	-0.894310000	1.548991000	2.010699000
Sn	-1.278216000	2.213936000	-1.202234000

3.3.4. $[Cu@Sn_{10}]^{0}$ / $^2E_1$ / E = –1.37269028 au / $\langle S^2 \rangle$ = 0.75273

Cu	0.000000000	0.000000000	-0.104935000
Sn	1.810651000	0.000000000	2.032264000
Sn	-0.905325000	-1.568070000	2.032264000
Sn	2.571869000	0.000000000	-1.212112000
Sn	0.000000000	0.000000000	-2.791493000
Sn	-2.798156000	0.000000000	0.107151000
Sn	1.399078000	2.423274000	0.107151000
Sn	-1.285935000	-2.227304000	-1.212112000
Sn	1.399078000	-2.423274000	0.107151000
Sn	-0.905325000	1.568070000	2.032264000
Sn	-1.285935000	2.227304000	-1.212112000

3.3.5. $[Zn@Sn_{10}]^{1+}$ / $^2E_1$ / E = –1.11290564 au / $\langle S^2 \rangle$ = 0.75316

Zn	0.000000000	0.000000000	-0.100356000
Sn	1.836891000	0.000000000	2.060354000
Sn	-0.918445000	-1.590794000	2.060354000
Sn	2.608051000	0.000000000	-1.223300000
Sn	0.000000000	0.000000000	-2.858752000
Sn	-2.840120000	0.000000000	0.112922000
Sn	1.420060000	2.459616000	0.112922000
Sn	-1.304026000	-2.258639000	-1.223300000
Sn	1.420060000	-2.459616000	0.112922000
Sn	-0.918445000	1.590794000	2.060354000
Sn	-1.304026000	2.258639000	-1.223300000

3.4. *nido*-Octadecahedron (C_{2v})

3.4.1. $[Fe@Sn_{10}]^{3-}$ / $^2A_2$ / E = –1.91909020 au / $\langle S^2 \rangle$ = 0.94232

Fe	0.000000000	0.000000000	-0.026687000
Sn	-1.542225000	0.000000000	-2.180308000
Sn	1.542225000	0.000000000	-2.180308000
Sn	-1.508882000	-2.421948000	-0.521848000
Sn	1.508882000	-2.421948000	-0.521848000
Sn	-2.473941000	0.000000000	1.065195000
Sn	1.508882000	2.421948000	-0.521848000
Sn	0.000000000	1.546107000	2.165644000
Sn	0.000000000	-1.546107000	2.165644000
Sn	-1.508882000	2.421948000	-0.521848000
Sn	2.473941000	0.000000000	1.065195000

3.4.2. $[Co@Sn_{10}]^{2-}$/ $^2A_2$ / E = –1.80609554 au / $\langle S^2 \rangle$ = 0.76988

Co	0.000000000	0.000000000	0.068899000
Sn	-2.466299000	0.000000000	-1.080503000
Sn	-1.536710000	0.000000000	2.220425000
Sn	1.498054000	2.374506000	0.510588000
Sn	0.000000000	1.530758000	-2.180953000
Sn	-1.498054000	2.374506000	0.510588000
Sn	-1.498054000	-2.374506000	0.510588000
Sn	1.536710000	0.000000000	2.220425000
Sn	2.466299000	0.000000000	-1.080503000
Sn	0.000000000	-1.530758000	-2.180953000
Sn	1.498054000	-2.374506000	0.510588000

3.4.3. $[Ni@Sn_{10}]^{1-}$ / $^2A_2$ / E = –1.60298667 au / $\langle S^2 \rangle$ = 0.75268

Ni	0.000000000	0.000000000	0.092829000
Sn	-2.473501000	0.000000000	-1.088178000
Sn	-1.550058000	0.000000000	2.255232000
Sn	1.495096000	2.360103000	0.504426000
Sn	0.000000000	1.534308000	-2.201348000
Sn	-1.495096000	2.360103000	0.504426000
Sn	-1.495096000	-2.360103000	0.504426000
Sn	1.550058000	0.000000000	2.255232000
Sn	2.473501000	0.000000000	-1.088178000
Sn	0.000000000	-1.534308000	-2.201348000
Sn	1.495096000	-2.360103000	0.504426000

3.4.4. $[Cu@Sn_{10}]^{0}$/ $^2A_2$ / E = –1.37881333 au / $\langle S^2 \rangle$ = 0.75284

Cu	0.000000000	0.000000000	0.098776000
Sn	-2.498235000	0.000000000	-1.094135000
Sn	-1.583028000	0.000000000	2.287237000
Sn	1.509344000	2.378339000	0.504482000
Sn	0.000000000	1.547437000	-2.230543000
Sn	-1.509344000	2.378339000	0.504482000
Sn	-1.509344000	-2.378339000	0.504482000
Sn	1.583028000	0.000000000	2.287237000
Sn	2.498235000	0.000000000	-1.094135000
Sn	0.000000000	-1.547437000	-2.230543000
Sn	1.509344000	-2.378339000	0.504482000

3.4.5. $[Zn@Sn_{10}]^{1+}$ / $^2A_2$ / E = –1.11956933 au / $\langle S^2 \rangle$ = 0.75330

Zn	0.000000000	0.000000000	0.095930000
Sn	-2.539265000	0.000000000	-1.101051000
Sn	-1.633087000	0.000000000	2.323774000
Sn	1.534949000	2.410600000	0.505917000
Sn	0.000000000	1.567673000	-2.262594000
Sn	-1.534949000	2.410600000	0.505917000
Sn	-1.534949000	-2.410600000	0.505917000
Sn	1.633087000	0.000000000	2.323774000
Sn	2.539265000	0.000000000	-1.101051000
Sn	0.000000000	-1.567673000	-2.262594000
Sn	1.534949000	-2.410600000	0.505917000

3.5. C_2-symmetric geometry

3.5.1. $[Fe@Sn_{10}]^{3-}$ / ^2A / E = –1.92079336 au / $\langle S^2 \rangle$ = 0.87788

Fe	0.000000000	0.000000000	-0.036529000
Sn	-0.651573000	1.413167000	2.167479000
Sn	-2.246145000	-1.010736000	1.064012000
Sn	0.651573000	-1.413167000	2.167479000
Sn	2.246145000	1.010736000	1.064012000
Sn	0.431482000	3.037897000	-0.378673000
Sn	-2.155001000	1.529525000	-0.644549000
Sn	-1.241120000	-0.879757000	-2.199747000
Sn	-0.431482000	-3.037897000	-0.378673000
Sn	2.155001000	-1.529525000	-0.644549000
Sn	1.241120000	0.879757000	-2.199747000

4. Tin clusters, Total Valence Electron Count 52 (S = 0)

4.1. Pentagonal Prismatic (D_{5h})

4.1.1. $[Fe@Sn_{10}]^{4-}$ / $^1A_1'$ / E = –1.99563925 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	0.000000000
Sn	0.754921000	-2.323407000	-1.489653000
Sn	-1.976408000	-1.435944000	-1.489653000
Sn	-1.976408000	1.435944000	-1.489653000
Sn	0.754921000	2.323407000	-1.489653000
Sn	2.442975000	0.000000000	-1.489653000
Sn	0.754921000	-2.323407000	1.489653000
Sn	-1.976408000	-1.435944000	1.489653000
Sn	-1.976408000	1.435944000	1.489653000
Sn	0.754921000	2.323407000	1.489653000
Sn	2.442975000	0.000000000	1.489653000

4.1.2. $[Co@Sn_{10}]^{3-}$ / $^1A_1'$ / E = –1.88650627 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	0.000000000
Sn	0.754238000	-2.321306000	-1.487043000
Sn	-1.974621000	-1.434646000	-1.487043000
Sn	-1.974621000	1.434646000	-1.487043000
Sn	0.754238000	2.321306000	-1.487043000

Sn	2.440766000	0.000000000	-1.487043000
Sn	0.754238000	-2.321306000	1.487043000
Sn	-1.974621000	-1.434646000	1.487043000
Sn	-1.974621000	1.434646000	1.487043000
Sn	0.754238000	2.321306000	1.487043000
Sn	2.440766000	0.000000000	1.487043000

4.1.3. $[Ni@Sn_{10}]^{2-}$ / $^1A_1'$ / E = –1.68835654 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	0.000000000
Sn	0.757343000	-2.330862000	-1.491486000
Sn	-1.982750000	-1.440552000	-1.491486000
Sn	-1.982750000	1.440552000	-1.491486000
Sn	0.757343000	2.330862000	-1.491486000
Sn	2.450813000	0.000000000	-1.491486000
Sn	0.757343000	-2.330862000	1.491486000
Sn	-1.982750000	-1.440552000	1.491486000
Sn	-1.982750000	1.440552000	1.491486000
Sn	0.757343000	2.330862000	1.491486000
Sn	2.450813000	0.000000000	1.491486000

4.1.4. $[Cu@Sn_{10}]^{1-}$ / $^1A_1'$ / E = –1.47105684 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	0.000000000
Sn	0.764952000	-2.354279000	-1.502572000
Sn	-2.002669000	-1.455024000	-1.502572000
Sn	-2.002669000	1.455024000	-1.502572000
Sn	0.764952000	2.354279000	-1.502572000
Sn	2.475435000	0.000000000	-1.502572000
Sn	0.764952000	-2.354279000	1.502572000
Sn	-2.002669000	-1.455024000	1.502572000
Sn	-2.002669000	1.455024000	1.502572000
Sn	0.764952000	2.354279000	1.502572000
Sn	2.475435000	0.000000000	1.502572000

4.1.5. $[Zn@Sn_{10}]^{0}$ / $^1A_1'$ / E = –1.22414697 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	0.000000000
Sn	0.775282000	-2.386073000	-1.520868000
Sn	-2.029715000	-1.474674000	-1.520868000
Sn	-2.029715000	1.474674000	-1.520868000
Sn	0.775282000	2.386073000	-1.520868000
Sn	2.508866000	0.000000000	-1.520868000
Sn	0.775282000	-2.386073000	1.520868000
Sn	-2.029715000	-1.474674000	1.520868000
Sn	-2.029715000	1.474674000	1.520868000
Sn	0.775282000	2.386073000	1.520868000
Sn	2.508866000	0.000000000	1.520868000

4.2. Bicapped Square Antiprismatic (D_{4d})

4.2.1. $[Fe@Sn_{10}]^{4-}$ / $^1A_1$ / E = –1.99416945 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	0.000000000
Sn	0.944167000	-2.279421000	1.164698000
Sn	2.279421000	0.944167000	1.164698000

Sn	-0.944167000	2.279421000	1.164698000
Sn	-2.279421000	-0.944167000	1.164698000
Sn	0.000000000	0.000000000	2.870915000
Sn	2.279421000	-0.944167000	-1.164698000
Sn	0.944167000	2.279421000	-1.164698000
Sn	-2.279421000	0.944167000	-1.164698000
Sn	-0.944167000	-2.279421000	-1.164698000
Sn	0.000000000	0.000000000	-2.870915000

4.2.2. $[Co@Sn_{10}]^{3-}$ / $^{1}A_{1}$ / E = –1.90980858 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	0.000000000
Sn	0.902731000	-2.179384000	1.231661000
Sn	2.179384000	0.902731000	1.231661000
Sn	-0.902731000	2.179384000	1.231661000
Sn	-2.179384000	-0.902731000	1.231661000
Sn	0.000000000	0.000000000	3.121836000
Sn	2.179384000	-0.902731000	-1.231661000
Sn	0.902731000	2.179384000	-1.231661000
Sn	-2.179384000	0.902731000	-1.231661000
Sn	-0.902731000	-2.179384000	-1.231661000
Sn	0.000000000	0.000000000	-3.121836000

4.2.3. $[Ni@Sn_{10}]^{2-}$ / $^{1}A_{1}$ / E = –1.73679807 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	0.000000000
Sn	0.901046000	-2.175318000	1.247247000
Sn	2.175318000	0.901046000	1.247247000
Sn	-0.901046000	2.175318000	1.247247000
Sn	-2.175318000	-0.901046000	1.247247000
Sn	0.000000000	0.000000000	3.169587000
Sn	2.175318000	-0.901046000	-1.247247000
Sn	0.901046000	2.175318000	-1.247247000
Sn	-2.175318000	0.901046000	-1.247247000
Sn	-0.901046000	-2.175318000	-1.247247000
Sn	0.000000000	0.000000000	-3.169587000

4.2.4. $[Cu@Sn_{10}]^{1-}$ / $^{1}A_{1}$ / E = –1.53405869 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	0.000000000
Sn	0.916223000	-2.211958000	1.248772000
Sn	2.211958000	0.916223000	1.248772000
Sn	-0.916223000	2.211958000	1.248772000
Sn	-2.211958000	-0.916223000	1.248772000
Sn	0.000000000	0.000000000	3.167037000
Sn	2.211958000	-0.916223000	-1.248772000
Sn	0.916223000	2.211958000	-1.248772000
Sn	-2.211958000	0.916223000	-1.248772000
Sn	-0.916223000	-2.211958000	-1.248772000
Sn	0.000000000	0.000000000	-3.167037000

4.2.5. $[Zn@Sn_{10}]^{0}$ / $^{1}A_{1}$ / E = –1.28971585 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	0.000000000
Sn	0.934323000	-2.255654000	1.264077000
Sn	2.255654000	0.934323000	1.264077000
Sn	-0.934323000	2.255654000	1.264077000
Sn	-2.255654000	-0.934323000	1.264077000

Sn	0.000000000	0.000000000	3.174564000
Sn	2.255654000	-0.934323000	-1.264077000
Sn	0.934323000	2.255654000	-1.264077000
Sn	-2.255654000	0.934323000	-1.264077000
Sn	-0.934323000	-2.255654000	-1.264077000
Sn	0.000000000	0.000000000	-3.174564000

4.3.Tetracapped Trigonal Prismatic (C_{3v})

4.3.1. $[Fe@Sn_{10}]^{4-}$ / $^{1}A_1$ / E = –1.99569355 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	0.230650000
Sn	1.782927000	0.000000000	2.359991000
Sn	-0.891463000	-1.544060000	2.359991000
Sn	1.893919000	0.000000000	-1.563351000
Sn	0.000000000	0.000000000	-3.913427000
Sn	-2.654559000	0.000000000	0.444994000
Sn	1.327280000	2.298916000	0.444994000
Sn	-0.946959000	-1.640182000	-1.563351000
Sn	1.327280000	-2.298916000	0.444994000
Sn	-0.891463000	1.544060000	2.359991000
Sn	-0.946959000	1.640182000	-1.563351000

4.3.2. $[Co@Sn_{10}]^{3-}$ / $^{1}A_1$ / E = –1.89786821 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	0.272511000
Sn	1.787554000	0.000000000	2.273031000
Sn	-0.893777000	-1.548067000	2.273031000
Sn	1.909877000	0.000000000	-1.455620000
Sn	0.000000000	0.000000000	-3.795969000
Sn	-2.728045000	0.000000000	0.378613000
Sn	1.364023000	2.362557000	0.378613000
Sn	-0.954938000	-1.654002000	-1.455620000
Sn	1.364023000	-2.362557000	0.378613000
Sn	-0.893777000	1.548067000	2.273031000
Sn	-0.954938000	1.654002000	-1.455620000

4.3.3. $[Ni@Sn_{10}]^{2-}$ / $^{1}A_1$ / E = –1.71233588 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	0.296167000
Sn	1.792075000	0.000000000	2.252975000
Sn	-0.896038000	-1.551983000	2.252975000
Sn	1.924137000	0.000000000	-1.421135000
Sn	0.000000000	0.000000000	-3.754441000
Sn	-2.777778000	0.000000000	0.346514000
Sn	1.388889000	2.405626000	0.346514000
Sn	-0.962068000	-1.666351000	-1.421135000
Sn	1.388889000	-2.405626000	0.346514000
Sn	-0.896038000	1.551983000	2.252975000
Sn	-0.962068000	1.666351000	-1.421135000

4.3.4. $[Cu@Sn_{10}]^{1-}$ / $^{1}A_1$ / E = –1.50095583 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	0.303217000
Sn	1.802136000	0.000000000	2.282381000
Sn	-0.901068000	-1.560695000	2.282381000
Sn	1.959456000	0.000000000	-1.432288000
Sn	0.000000000	0.000000000	-3.748795000

Sn	-2.809304000	0.000000000	0.324906000
Sn	1.404652000	2.432929000	0.324906000
Sn	-0.979728000	-1.696939000	-1.432288000
Sn	1.404652000	-2.432929000	0.324906000
Sn	-0.901068000	1.560695000	2.282381000
Sn	-0.979728000	1.696939000	-1.432288000

4.3.5. $[Zn@Sn_{10}]^{0}$ / $^{1}A_{1}$ / E = –1.25143324 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	0.317372000
Sn	1.821790000	0.000000000	2.342717000
Sn	-0.910895000	-1.577716000	2.342717000
Sn	2.004799000	0.000000000	-1.465467000
Sn	0.000000000	0.000000000	-3.773328000
Sn	-2.836024000	0.000000000	0.303343000
Sn	1.418012000	2.456069000	0.303343000
Sn	-1.002400000	-1.736207000	-1.465467000
Sn	1.418012000	-2.456069000	0.303343000
Sn	-0.910895000	1.577716000	2.342717000
Sn	-1.002400000	1.736207000	-1.465467000

4.4. *nido*-Octadecahedron (C_{2v})

4.4.1. $[Fe@Sn_{10}]^{4-}$ / $^{1}A_{1}$ / E = –2.00205396 au / $\langle S^2 \rangle$ = 0.00000

Fe	0.000000000	0.000000000	-0.034049000
Sn	-2.592096000	0.000000000	1.035309000
Sn	0.000000000	1.510282000	2.134448000
Sn	1.547615000	2.361068000	-0.484728000
Sn	-1.588901000	0.000000000	-2.182848000
Sn	-1.547615000	2.361068000	-0.484728000
Sn	0.000000000	-1.510282000	2.134448000
Sn	2.592096000	0.000000000	1.035309000
Sn	1.588901000	0.000000000	-2.182848000
Sn	-1.547615000	-2.361068000	-0.484728000
Sn	1.547615000	-2.361068000	-0.484728000

4.4.2. $[Co@Sn_{10}]^{3-}$ / $^{1}A_{1}$ / E = –1.90703249 au / $\langle S^2 \rangle$ = 0.00000

Co	0.000000000	0.000000000	-0.049613000
Sn	-2.510952000	0.000000000	1.036518000
Sn	0.000000000	1.518438000	2.153134000
Sn	1.529226000	2.389674000	-0.500702000
Sn	-1.593052000	0.000000000	-2.167363000
Sn	-1.529226000	2.389674000	-0.500702000
Sn	0.000000000	-1.518438000	2.153134000
Sn	2.510952000	0.000000000	1.036518000
Sn	1.593052000	0.000000000	-2.167363000
Sn	-1.529226000	-2.389674000	-0.500702000
Sn	1.529226000	-2.389674000	-0.500702000

4.4.3. $[Ni@Sn_{10}]^{2-}$ / $^{1}A_{1}$ / E = –1.72335390 au / $\langle S^2 \rangle$ = 0.00000

Ni	0.000000000	0.000000000	-0.072336000
Sn	-2.486404000	0.000000000	1.029337000
Sn	0.000000000	1.528246000	2.174111000

Sn	1.532524000	2.414734000	-0.505002000
Sn	-1.616894000	0.000000000	-2.167003000
Sn	-1.532524000	2.414734000	-0.505002000
Sn	0.000000000	-1.528246000	2.174111000
Sn	2.486404000	0.000000000	1.029337000
Sn	1.616894000	0.000000000	-2.167003000
Sn	-1.532524000	-2.414734000	-0.505002000
Sn	1.532524000	-2.414734000	-0.505002000

4.4.4. $[Cu@Sn_{10}]^{1-}$ / $^1A_1$ / E = –1.51635982 au / $\langle S^2 \rangle$ = 0.00000

Cu	0.000000000	0.000000000	-0.099522000
Sn	-2.497668000	0.000000000	1.031050000
Sn	0.000000000	1.545730000	2.199566000
Sn	1.551644000	2.439836000	-0.505330000
Sn	-1.670628000	0.000000000	-2.186240000
Sn	-1.551644000	2.439836000	-0.505330000
Sn	0.000000000	-1.545730000	2.199566000
Sn	2.497668000	0.000000000	1.031050000
Sn	1.670628000	0.000000000	-2.186240000
Sn	-1.551644000	-2.439836000	-0.505330000
Sn	1.551644000	-2.439836000	-0.505330000

4.4.5. $[Zn@Sn_{10}]^{0}$ / $^1A_1$ / E = –1.27267674 au / $\langle S^2 \rangle$ = 0.00000

Zn	0.000000000	0.000000000	-0.143540000
Sn	-2.524896000	0.000000000	1.042182000
Sn	0.000000000	1.556453000	2.232367000
Sn	1.581989000	2.472123000	-0.505795000
Sn	-1.764077000	0.000000000	-2.217367000
Sn	-1.581989000	2.472123000	-0.505795000
Sn	0.000000000	-1.556453000	2.232367000
Sn	2.524896000	0.000000000	1.042182000
Sn	1.764077000	0.000000000	-2.217367000
Sn	-1.581989000	-2.472123000	-0.505795000
Sn	1.581989000	-2.472123000	-0.505795000

5. Indium and Lead clusters, Total Valence Electron Count 50/52

5.1. $[Ni@In_{10}]^{10-}$, 50VE

5.1.1. $[Ni@In_{10}]^{10-}$, Pentagonal Prismatic (D_{5h}) - triplet

Ni	0.000000000	0.000000000	0.000000000
In	2.511110000	0.000000000	-1.482822000
In	2.511110000	0.000000000	1.482822000
In	0.775976000	2.388208000	1.482822000
In	0.775976000	-2.388208000	1.482822000
In	0.775976000	2.388208000	-1.482822000
In	0.775976000	-2.388208000	-1.482822000
In	-2.031531000	1.475994000	1.482822000
In	-2.031531000	-1.475994000	1.482822000
In	-2.031531000	1.475994000	-1.482822000
In	-2.031531000	-1.475994000	-1.482822000

5.1.2. $[Ni@In_{10}]^{10-}$, Bicapped Square Antiprismatic (D_{4d}) - singlet

Ni	0.000000000	0.000000000	0.000000000
In	0.000000000	0.000000000	-2.830280000
In	0.000000000	0.000000000	2.830280000
In	2.323145000	0.962278000	-1.182610000
In	-0.962278000	2.323145000	-1.182610000
In	-2.323145000	-0.962278000	-1.182610000
In	0.962278000	-2.323145000	-1.182610000
In	2.323145000	-0.962278000	1.182610000
In	-0.962278000	-2.323145000	1.182610000
In	-2.323145000	0.962278000	1.182610000
In	0.962278000	2.323145000	1.182610000

5.1.3. $[Ni@In_{10}]^{10-}$, Tetracapped Trigonal Prismatic (C_{3v}) - singlet

Ni	0.000000000	0.000000000	-0.073701000
In	1.264972000	-2.190996000	-1.218156000
In	0.000000000	0.000000000	-2.821086000
In	2.795343000	0.000000000	0.114705000
In	1.264972000	2.190996000	-1.218156000
In	0.916589000	-1.587579000	2.062406000
In	-2.529945000	0.000000000	-1.218156000
In	-1.833178000	0.000000000	2.062406000
In	0.916589000	1.587579000	2.062406000
In	-1.397672000	-2.420838000	0.114705000
In	-1.397672000	2.420838000	0.114705000

5.1.4. $[Ni@In_{10}]^{10-}$, *nido*-Octadecahedron (C_{2v}) - singlet

Ni	0.000000000	0.000000000	-0.065458000
In	-1.496512000	0.000000000	-2.385122000
In	1.496512000	0.000000000	-2.385122000
In	-1.481895000	-2.314726000	-0.500787000
In	1.481895000	-2.314726000	-0.500787000
In	-2.523263000	0.000000000	1.142259000
In	1.481895000	2.314726000	-0.500787000
In	0.000000000	1.567616000	2.270660000
In	0.000000000	-1.567616000	2.270660000
In	-1.481895000	2.314726000	-0.500787000
In	2.523263000	0.000000000	1.142259000

5.2. $[Zn@In_{10}]^{8-}$, 50VE

5.2.1. $[Zn@In_{10}]^{8-}$, Pentagonal Prismatic (D_{5h}) - triplet

Zn	0.000000000	0.000000000	0.000000000
In	2.588112000	0.000000000	-1.510164000
In	2.588112000	0.000000000	1.510164000
In	0.799770000	2.461440000	1.510164000
In	0.799770000	-2.461440000	1.510164000
In	0.799770000	2.461440000	-1.510164000
In	0.799770000	-2.461440000	-1.510164000
In	-2.093826000	1.521254000	1.510164000
In	-2.093826000	-1.521254000	1.510164000
In	-2.093826000	1.521254000	-1.510164000
In	-2.093826000	-1.521254000	-1.510164000

5.2.2. $[Zn@In_{10}]^{8-}$, Bicapped Square Antiprismatic (D_{4d}) - singlet

Zn	0.000000000	0.000000000	0.000000000
In	0.000000000	0.000000000	-2.874647000
In	0.000000000	0.000000000	2.874647000
In	0.993330000	2.398111000	-1.219221000
In	2.398111000	-0.993330000	-1.219221000
In	-2.398111000	0.993330000	-1.219221000
In	-0.993330000	-2.398111000	-1.219221000
In	2.398111000	0.993330000	1.219221000
In	-0.993330000	2.398111000	1.219221000
In	0.993330000	-2.398111000	1.219221000
In	-2.398111000	-0.993330000	1.219221000

5.2.3. $[Zn@In_{10}]^{8-}$, Tetracapped Trigonal Prismatic (C_{3v}) - singlet

Zn	0.000000000	0.000000000	-0.059189000
In	1.295487000	-2.243850000	-1.256294000
In	0.000000000	0.000000000	-2.929609000
In	2.863193000	0.000000000	0.127632000
In	1.295487000	2.243850000	-1.256294000
In	0.941915000	-1.631444000	2.118953000
In	-2.590975000	0.000000000	-1.256294000
In	-1.883829000	0.000000000	2.118953000
In	0.941915000	1.631444000	2.118953000
In	-1.431597000	-2.479598000	0.127632000
In	-1.431597000	2.479598000	0.127632000

5.2.4. $[Zn@In_{10}]^{8-}$, *nido*-Octadecahedron (C_{2v}) - singlet

Zn	0.000000000	0.000000000	-0.051713000
In	-1.551882000	0.000000000	-2.460015000
In	1.551882000	0.000000000	-2.460015000
In	-1.524918000	-2.374429000	-0.519948000
In	1.524918000	-2.374429000	-0.519948000
In	-2.596892000	0.000000000	1.190589000
In	1.524918000	2.374429000	-0.519948000
In	0.000000000	1.617894000	2.328673000
In	0.000000000	-1.617894000	2.328673000
In	-1.524918000	2.374429000	-0.519948000
In	2.596892000	0.000000000	1.190589000

5.3. $[Ni@Pb_{10}]^{2-}$, 52VE

5.3.1. $[Ni@Pb_{10}]^{2-}$, Pentagonal Prismatic (D_{5h}) - singlet

Ni	0.000000000	0.000000000	0.000000000
Pb	2.569505000	0.000000000	-1.573214000
Pb	2.569505000	0.000000000	1.573214000
Pb	0.794021000	2.443744000	1.573214000
Pb	0.794021000	-2.443744000	1.573214000
Pb	0.794021000	2.443744000	-1.573214000
Pb	0.794021000	-2.443744000	-1.573214000
Pb	-2.078773000	1.510317000	1.573214000
Pb	-2.078773000	-1.510317000	1.573214000
Pb	-2.078773000	1.510317000	-1.573214000
Pb	-2.078773000	-1.510317000	-1.573214000

5.3.2. $[Ni@Pb_{10}]^{2-}$, Bicapped Square Antiprismatic (D_{4d}) - singlet

Ni	0.000000000	0.000000000	0.000000000
Pb	0.000000000	0.000000000	-3.396681000

Pb	0.000000000	0.000000000	3.396681000
Pb	0.930281000	2.245898000	-1.336778000
Pb	2.245898000	-0.930281000	-1.336778000
Pb	-2.245898000	0.930281000	-1.336778000
Pb	-0.930281000	-2.245898000	-1.336778000
Pb	2.245898000	0.930281000	1.336778000
Pb	-0.930281000	2.245898000	1.336778000
Pb	0.930281000	-2.245898000	1.336778000
Pb	-2.245898000	-0.930281000	1.336778000

5.3.3. $[Ni@Pb_{10}]^{2-}$, Tetracapped Trigonal Prismatic (C_{3v}) - triplet

Ni	0.000000000	0.000000000	-0.088325000
Pb	1.396636000	-2.419044000	-1.189919000
Pb	0.000000000	0.000000000	-2.750472000
Pb	2.934218000	0.000000000	0.073591000
Pb	1.396636000	2.419044000	-1.189919000
Pb	0.942451000	-1.632373000	2.056620000
Pb	-2.793272000	0.000000000	-1.189919000
Pb	-1.884902000	0.000000000	2.056620000
Pb	0.942451000	1.632373000	2.056620000
Pb	-1.467109000	-2.541107000	0.073591000
Pb	-1.467109000	2.541107000	0.073591000

5.3.4. $[Ni@Pb_{10}]^{2-}$, *nido*-Octadecahedron (C_{2v}) - singlet

Ni	0.000000000	0.000000000	-0.100574000
Pb	-1.743360000	0.000000000	-2.239488000
Pb	1.743360000	0.000000000	-2.239488000
Pb	-1.599927000	-2.558777000	-0.511361000
Pb	1.599927000	-2.558777000	-0.511361000
Pb	-2.611281000	0.000000000	1.064085000
Pb	1.599927000	2.558777000	-0.511361000
Pb	0.000000000	1.610218000	2.241905000
Pb	0.000000000	-1.610218000	2.241905000
Pb	-1.599927000	2.558777000	-0.511361000
Pb	2.611281000	0.000000000	1.064085000

6. Vacant shell clusters

6.1. Indium, 40VE

6.1.1. $[In_{10}]^{10-}$, Pentagonal Prismatic (D_{5h})

In	2.539278000	0.000000000	-1.482806000
In	2.539278000	0.000000000	1.482806000
In	0.784680000	2.414997000	1.482806000
In	0.784680000	-2.414997000	1.482806000
In	0.784680000	2.414997000	-1.482806000
In	0.784680000	-2.414997000	-1.482806000
In	-2.054319000	1.492550000	1.482806000
In	-2.054319000	-1.492550000	1.482806000
In	-2.054319000	1.492550000	-1.482806000
In	-2.054319000	-1.492550000	-1.482806000

6.1.2. $[In_{10}]^{10-}$, Bicapped Square Antiprismatic (D_{4d})

In	0.000000000	0.000000000	-2.798742000
In	0.000000000	0.000000000	2.798742000
In	0.949291000	2.291791000	-1.177802000

In	2.291791000	-0.949291000	-1.177802000
In	-2.291791000	0.949291000	-1.177802000
In	-0.949291000	-2.291791000	-1.177802000
In	2.291791000	0.949291000	1.177802000
In	-0.949291000	2.291791000	1.177802000
In	0.949291000	-2.291791000	1.177802000
In	-2.291791000	-0.949291000	1.177802000

6.1.3. $[In_{10}]^{10-}$, Tetracapped Trigonal Prismatic (C_{3v})

In	1.000684000	-1.733236000	-1.164314000
In	0.000000000	0.000000000	-3.348852000
In	3.045608000	0.000000000	0.325613000
In	1.000684000	1.733236000	-1.164314000
In	0.914608000	-1.584148000	1.973580000
In	-2.001369000	0.000000000	-1.164314000
In	-1.829216000	0.000000000	1.973580000
In	0.914608000	1.584148000	1.973580000
In	-1.522804000	-2.637574000	0.325613000
In	-1.522804000	2.637574000	0.325613000

6.1.4. $[In_{10}]^{10-}$, *nido*-Octadecahedron (C_{2v})

In	-1.501293000	0.000000000	-2.350572000
In	1.501293000	0.000000000	-2.350572000
In	-1.469808000	-2.305597000	-0.501565000
In	1.469808000	-2.305597000	-0.501565000
In	-2.491566000	0.000000000	1.117882000
In	1.469808000	2.305597000	-0.501565000
In	0.000000000	1.555843000	2.241495000
In	0.000000000	-1.555843000	2.241495000
In	-1.469808000	2.305597000	-0.501565000
In	2.491566000	0.000000000	1.117882000

6.2. Indium, 42VE

6.2.1. $[In_{10}]^{12-}$, Pentagonal Prismatic (D_{5h})

In	2.563051000	0.000000000	-1.541884000
In	2.563051000	0.000000000	1.541884000
In	0.792026000	2.437607000	1.541884000
In	0.792026000	-2.437607000	1.541884000
In	0.792026000	2.437607000	-1.541884000
In	0.792026000	-2.437607000	-1.541884000
In	-2.073552000	1.506524000	1.541884000
In	-2.073552000	-1.506524000	1.541884000
In	-2.073552000	1.506524000	-1.541884000
In	-2.073552000	-1.506524000	-1.541884000

6.2.2. $[In_{10}]^{12-}$, Bicapped Square Antiprismatic (D_{4d})

In	0.000000000	0.000000000	-3.250357000
In	0.000000000	0.000000000	3.250357000
In	0.892270000	2.154130000	-1.245447000
In	2.154130000	-0.892270000	-1.245447000
In	-2.154130000	0.892270000	-1.245447000
In	-0.892270000	-2.154130000	-1.245447000
In	2.154130000	0.892270000	1.245447000
In	-0.892270000	2.154130000	1.245447000
In	0.892270000	-2.154130000	1.245447000
In	-2.154130000	-0.892270000	1.245447000

6.2.3. $[In_{10}]^{12-}$, Tetracapped Trigonal Prismatic (C_{3v})

In	1.397011000	-2.419694000	-1.172145000
In	0.000000000	0.000000000	-2.429086000
In	2.768264000	0.000000000	0.020763000
In	1.397011000	2.419694000	-1.172145000
In	0.908881000	-1.574228000	1.979672000
In	-2.794022000	0.000000000	-1.172145000
In	-1.817762000	0.000000000	1.979672000
In	0.908881000	1.574228000	1.979672000
In	-1.384132000	-2.397387000	0.020763000
In	-1.384132000	2.397387000	0.020763000

6.2.4. $[In_{10}]^{12-}$, *nido*-Octadecahedron (C_{2v})

In	-1.613433000	0.000000000	-2.122488000
In	1.613433000	0.000000000	-2.122488000
In	-1.576100000	-2.512952000	-0.499835000
In	1.576100000	-2.512952000	-0.499835000
In	-2.429446000	0.000000000	0.953089000
In	1.576100000	2.512952000	-0.499835000
In	0.000000000	1.561480000	2.174741000
In	0.000000000	-1.561480000	2.174741000
In	-1.576100000	2.512952000	-0.499835000
In	2.429446000	0.000000000	0.953089000

6.3.Indium, 44VE

6.3.1. $[In_{10}]^{14-}$, Pentagonal Prismatic (D_{5h})

In	2.541619000	0.000000000	-1.635453000
In	2.541619000	0.000000000	1.635453000
In	0.785404000	2.417224000	1.635453000
In	0.785404000	-2.417224000	1.635453000
In	0.785404000	2.417224000	-1.635453000
In	0.785404000	-2.417224000	-1.635453000
In	-2.056213000	1.493926000	1.635453000
In	-2.056213000	-1.493926000	1.635453000
In	-2.056213000	1.493926000	-1.635453000
In	-2.056213000	-1.493926000	-1.635453000

6.3.2. $[In_{10}]^{14-}$, Bicapped Square Antiprismatic (D_{4d})

In	0.000000000	0.000000000	-3.602038000
In	0.000000000	0.000000000	3.602038000
In	0.867364000	2.094003000	-1.302990000
In	2.094003000	-0.867364000	-1.302990000
In	-2.094003000	0.867364000	-1.302990000
In	-0.867364000	-2.094003000	-1.302990000
In	2.094003000	0.867364000	1.302990000
In	-0.867364000	2.094003000	1.302990000
In	0.867364000	-2.094003000	1.302990000
In	-2.094003000	-0.867364000	1.302990000

6.3.3. $[In_{10}]^{14-}$, Tetracapped Trigonal Prismatic (C_{3v})

In	1.412830000	-2.447093000	-1.130940000
In	0.000000000	0.000000000	-2.411649000

In	2.924525000	0.000000000	0.062354000
In	1.412830000	2.447093000	-1.130940000
In	0.914398000	-1.583785000	1.891064000
In	-2.825660000	0.000000000	-1.130940000
In	-1.828797000	0.000000000	1.891064000
In	0.914398000	1.583785000	1.891064000
In	-1.462262000	-2.532713000	0.062354000
In	-1.462262000	2.532713000	0.062354000

6.3.4. $[In_{10}]^{14-}$, *nido*-Octadecahedron (C_{2v})

In	-1.502970000	0.000000000	-2.132668000
In	1.502970000	0.000000000	-2.132668000
In	-1.569635000	-2.692468000	-0.405087000
In	1.569635000	-2.692468000	-0.405087000
In	-2.481389000	0.000000000	0.822198000
In	1.569635000	2.692468000	-0.405087000
In	0.000000000	1.543158000	2.126317000
In	0.000000000	-1.543158000	2.126317000
In	-1.569635000	2.692468000	-0.405087000
In	2.481389000	0.000000000	0.822198000

6.4.Tin, 40VE

6.4.1. $[Sn_{10}]$, Pentagonal Prismatic (D_{5h})

Sn	2.463526000	0.000000000	-1.445840000
Sn	2.463526000	0.000000000	1.445840000
Sn	0.761271000	2.342952000	1.445840000
Sn	0.761271000	-2.342952000	1.445840000
Sn	0.761271000	2.342952000	-1.445840000
Sn	0.761271000	-2.342952000	-1.445840000
Sn	-1.993034000	1.448024000	1.445840000
Sn	-1.993034000	-1.448024000	1.445840000
Sn	-1.993034000	1.448024000	-1.445840000
Sn	-1.993034000	-1.448024000	-1.445840000

6.4.2. $[Sn_{10}]$, Bicapped Square Antiprismatic (D_{4d})

Sn	0.000000000	0.000000000	-2.721046000
Sn	0.000000000	0.000000000	2.721046000
Sn	0.940396000	2.270317000	-1.164221000
Sn	2.270317000	-0.940396000	-1.164221000
Sn	-2.270317000	0.940396000	-1.164221000
Sn	-0.940396000	-2.270317000	-1.164221000
Sn	2.270317000	0.940396000	1.164221000
Sn	-0.940396000	2.270317000	1.164221000
Sn	0.940396000	-2.270317000	1.164221000
Sn	-2.270317000	-0.940396000	1.164221000

6.4.3. $[Sn_{10}]$, Tetracapped Trigonal Prismatic (C_{3v})

Sn	0.969562000	-1.679331000	-1.137303000
Sn	0.000000000	0.000000000	-3.324306000
Sn	3.010987000	0.000000000	0.324139000
Sn	0.969562000	1.679331000	-1.137303000
Sn	0.898064000	-1.555492000	1.939861000
Sn	-1.939124000	0.000000000	-1.137303000
Sn	-1.796127000	0.000000000	1.939861000

Sn	0.898064000	1.555492000	1.939861000
Sn	-1.505494000	-2.607592000	0.324139000
Sn	-1.505494000	2.607592000	0.324139000

6.4.4. $[Sn_{10}]$, *nido*-Octadecahedron (C_{2v})

Sn	-1.479835000	0.000000000	-2.321243000
Sn	1.479835000	0.000000000	-2.321243000
Sn	-1.440383000	-2.260823000	-0.491988000
Sn	1.440383000	-2.260823000	-0.491988000
Sn	-2.467281000	0.000000000	1.102806000
Sn	1.440383000	2.260823000	-0.491988000
Sn	0.000000000	1.524750000	2.208086000
Sn	0.000000000	-1.524750000	2.208086000
Sn	-1.440383000	2.260823000	-0.491988000
Sn	2.467281000	0.000000000	1.102806000

6.5.Tin, 42VE

6.5.1. $[Sn_{10}]^{2-}$, Pentagonal Prismatic (D_{5h})

Sn	2.453983000	0.000000000	-1.486893000
Sn	2.453983000	0.000000000	1.486893000
Sn	0.758323000	2.333877000	1.486893000
Sn	0.758323000	-2.333877000	1.486893000
Sn	0.758323000	2.333877000	-1.486893000
Sn	0.758323000	-2.333877000	-1.486893000
Sn	-1.985314000	1.442415000	1.486893000
Sn	-1.985314000	-1.442415000	1.486893000
Sn	-1.985314000	1.442415000	-1.486893000
Sn	-1.985314000	-1.442415000	-1.486893000

6.5.2. $[Sn_{10}]^{2-}$, Bicapped Square Antiprismatic (D_{4d})

Sn	0.000000000	0.000000000	-3.183172000
Sn	0.000000000	0.000000000	3.183172000
Sn	0.877526000	2.118535000	-1.219633000
Sn	2.118535000	-0.877526000	-1.219633000
Sn	-2.118535000	0.877526000	-1.219633000
Sn	-0.877526000	-2.118535000	-1.219633000
Sn	2.118535000	0.877526000	1.219633000
Sn	-0.877526000	2.118535000	1.219633000
Sn	0.877526000	-2.118535000	1.219633000
Sn	-2.118535000	-0.877526000	1.219633000

6.5.3. $[Sn_{10}]^{2-}$, Tetracapped Trigonal Prismatic (C_{3v})

Sn	1.392816000	-2.412429000	-1.165641000
Sn	0.000000000	0.000000000	-2.304293000
Sn	2.649325000	0.000000000	-0.023023000
Sn	1.392816000	2.412429000	-1.165641000
Sn	0.888155000	-1.538330000	1.975356000
Sn	-2.785633000	0.000000000	-1.165641000
Sn	-1.776310000	0.000000000	1.975356000
Sn	0.888155000	1.538330000	1.975356000
Sn	-1.324663000	-2.294383000	-0.023023000
Sn	-1.324663000	2.294383000	-0.023023000

6.5.4. $[Sn_{10}]^{2-}$, *nido*-Octadecahedron (C_{2v})

Sn	-1.541668000	0.000000000	-2.086005000
Sn	1.541668000	0.000000000	-2.086005000
Sn	-1.523565000	-2.445619000	-0.505964000
Sn	1.523565000	-2.445619000	-0.505964000
Sn	-2.400067000	0.000000000	0.965522000
Sn	1.523565000	2.445619000	-0.505964000
Sn	0.000000000	1.521365000	2.138085000
Sn	0.000000000	-1.521365000	2.138085000
Sn	-1.523565000	2.445619000	-0.505964000
Sn	2.400067000	0.000000000	0.965522000

6.6.Tin, 44VE

6.6.1. $[Sn_{10}]^{4-}$, Pentagonal Prismatic (D_{5h})

Sn	2.502244000	0.000000000	-1.466337000
Sn	2.502244000	0.000000000	1.466337000
Sn	0.773236000	2.379776000	1.466337000
Sn	0.773236000	-2.379776000	1.466337000
Sn	0.773236000	2.379776000	-1.466337000
Sn	0.773236000	-2.379776000	-1.466337000
Sn	-2.024358000	1.470782000	1.466337000
Sn	-2.024358000	-1.470782000	1.466337000
Sn	-2.024358000	1.470782000	-1.466337000
Sn	-2.024358000	-1.470782000	-1.466337000

6.6.2. $[Sn_{10}]^{4-}$, Bicapped Square Antiprismatic (D_{4d})

Sn	0.000000000	0.000000000	-3.423495000
Sn	0.000000000	0.000000000	3.423495000
Sn	0.855287000	2.064847000	-1.260762000
Sn	2.064847000	-0.855287000	-1.260762000
Sn	-2.064847000	0.855287000	-1.260762000
Sn	-0.855287000	-2.064847000	-1.260762000
Sn	2.064847000	0.855287000	1.260762000
Sn	-0.855287000	2.064847000	1.260762000
Sn	0.855287000	-2.064847000	1.260762000
Sn	-2.064847000	-0.855287000	1.260762000

6.6.3. $[Sn_{10}]^{4-}$, Tetracapped Trigonal Prismatic (C_{3v})

Sn	1.371762000	-2.375961000	-1.086035000
Sn	0.000000000	0.000000000	-2.320790000
Sn	2.832515000	0.000000000	-0.001082000
Sn	1.371762000	2.375961000	-1.086035000
Sn	0.892448000	-1.545766000	1.879307000
Sn	-2.743523000	0.000000000	-1.086035000
Sn	-1.784896000	0.000000000	1.879307000
Sn	0.892448000	1.545766000	1.879307000
Sn	-1.416257000	-2.453030000	-0.001082000
Sn	-1.416257000	2.453030000	-0.001082000

6.6.4. $[Sn_{10}]^{4-}$, *nido*-Octadecahedron (C_{2v})

Sn	-1.469897000	0.000000000	-2.083580000
Sn	1.469897000	0.000000000	-2.083580000
Sn	-1.494398000	-2.561503000	-0.434753000
Sn	1.494398000	-2.561503000	-0.434753000
Sn	-2.435467000	0.000000000	0.859072000
Sn	1.494398000	2.561503000	-0.434753000

Sn	0.000000000	1.512703000	2.099688000
Sn	0.000000000	-1.512703000	2.099688000
Sn	-1.494398000	2.561503000	-0.434753000
Sn	2.435467000	0.000000000	0.859072000

6.7.Tin, 42VE

6.7.1. $[Pb_{10}]^{2-}$, Pentagonal Prismatic (D_{5h})

Pb	2.585022000	0.000000000	-1.578272000
Pb	2.585022000	0.000000000	1.578272000
Pb	0.798816000	2.458502000	1.578272000
Pb	0.798816000	-2.458502000	1.578272000
Pb	0.798816000	2.458502000	-1.578272000
Pb	0.798816000	-2.458502000	-1.578272000
Pb	-2.091327000	1.519438000	1.578272000
Pb	-2.091327000	-1.519438000	1.578272000
Pb	-2.091327000	1.519438000	-1.578272000
Pb	-2.091327000	-1.519438000	-1.578272000

6.7.2. $[Pb_{10}]^{2-}$, Bicapped Square Antiprismatic (D_{4d})

Pb	0.000000000	0.000000000	-3.375242000
Pb	0.000000000	0.000000000	3.375242000
Pb	0.917479000	2.214991000	-1.306513000
Pb	2.214991000	-0.917479000	-1.306513000
Pb	-2.214991000	0.917479000	-1.306513000
Pb	-0.917479000	-2.214991000	-1.306513000
Pb	2.214991000	0.917479000	1.306513000
Pb	-0.917479000	2.214991000	1.306513000
Pb	0.917479000	-2.214991000	1.306513000
Pb	-2.214991000	-0.917479000	1.306513000

6.7.3. $[Pb_{10}]^{2-}$, Tetracapped Trigonal Prismatic (C_{3v})

Pb	1.501080000	-2.599947000	-1.167190000
Pb	0.000000000	0.000000000	-2.392874000
Pb	2.812496000	0.000000000	-0.071822000
Pb	1.501080000	2.599947000	-1.167190000
Pb	0.936663000	-1.622348000	2.036130000
Pb	-3.002160000	0.000000000	-1.167190000
Pb	-1.873326000	0.000000000	2.036130000
Pb	0.936663000	1.622348000	2.036130000
Pb	-1.406248000	-2.435693000	-0.071822000
Pb	-1.406248000	2.435693000	-0.071822000

6.7.4. $[Pb_{10}]^{2-}$, *nido*-Octadecahedron (C_{2v})

Pb	-1.679510	0.000000	-2.183958
Pb	1.679510	0.000000	-2.183958
Pb	-1.596932	-2.587750	-0.515044
Pb	1.596932	-2.587750	-0.515044
Pb	-2.549324	0.000000	1.023190
Pb	1.596932	2.587750	-0.515044
Pb	0.000000	1.605344	2.227730
Pb	0.000000	-1.605344	2.227730
Pb	-1.596932	2.587750	-0.515044
Pb	2.549324	0.000000	1.023190

Complete reference 24a

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