Supplementary Information

Exploring Aromatic Rings with Planar Tetracoordinate Group 13-15 Elements

Dumer S. Sacanamboy,[a,b] Pamela L. Gamero-Begazo,[b] Kevin E. Parco-Valencia,[b] Diego Inostroza,[c] Lina Ruiz,[d] Luis Leyva-Parra,[e]* Gabriel Merino,[f]* and William Tiznado[a]*

[a] *Universidad Andrés Bello, Facultad de Ciencias Exactas, Departamento de Ciencias Químicas, Centro de Química Teórica & Computacional (CQT&C), Avenida República 275, 8370146 Santiago de Chile., Chile.* wtiznado@unab.cl

[b] *Doctorado en Fisicoquímica Molecular, Facultad de Ciencias Exactas, Universidad Andres Bello, República 275, Santiago de Chile, Chile.*

[c] *Laboratoire de Chimie Théorique, LCT, Sorbonne Université, CNRS, F-75005 Paris, France*

[d] *Instituto de Ciencias Biomédicas, Facultad de Ciencias de la Salud, Universidad Autónoma de Chile, Santiago de Chile, Chile.*

[e] *Facultad de Ingeniería y Arquitectura, Universidad Central de Chile (UCEN), Santa Isabel 1186, 8370146, Santiago, Chile.* luis.leyva@ucentral.cl

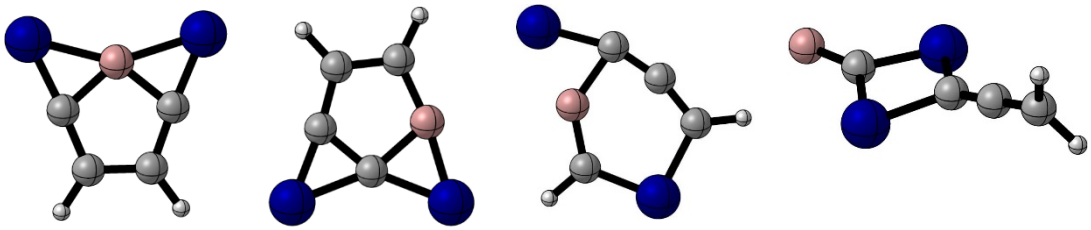
[f] *Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados Mérida Km. 6 Antigua carretera a Progreso Apdo. Postal 73, Cordemex, 97310, Mérida, Yuc., México.* gmerino@cinvestav.mx

Computational Details

We systematically explored the potential energy surface using AUTOMATON,[1] which employs probabilistic cellular automata to generate initial structures and genetic algorithms to evolve them towards the global minimum. Calculations for singlet and triplet states were performed at the PBE0[2]-D3[3]/SDDAll[4-8] level. The lowest energy structures (Figure S1-S18) were minimized at the PBE0-D3/def2-TZVP[9] level. For accurate energy comparisons, we conducted single-point energy calculations at the DLPNO-CCSD(T)[10-12]/CBS[13, 14]//PBE0-D3/def2-TZVP level via Gaussian 16 software.[15] Chemical bonding was analyzed using the Adaptive Natural Density Partitioning[16-18] (AdNDP) technique via Multiwfn software.[19] Structure and AdNDP orbitals were visualized using CYLview 2.0[20] and VMD 1.9.3.[21]

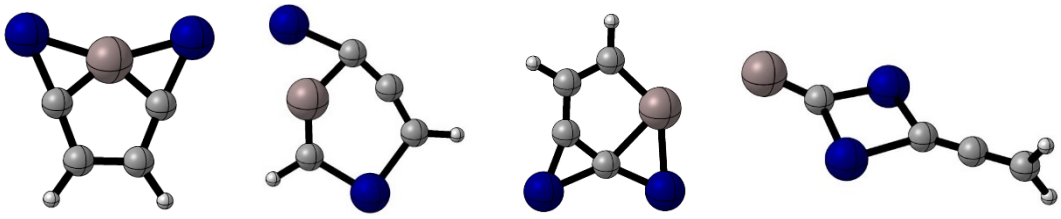
The Interacting Quantum Atoms (IQA) method[22-25] decomposed interaction energies, considering atomic deformation and interatomic interactions, and was performed at the PBE0-D3/def2-TZVP level using AIMAll.[26] The interaction energy (V_{IQA}^{int}) consists of Coulombic (V_C^{int}) and exchange-correlation (V_{XC}^{int}) terms, where V_C^{int} reflects electrostatic interaction between electrons and nuclei in a pair of basins, including nuclear repulsion, electron-nucleus attraction, and the Coulomb part of electron-electron repulsion. V_{XC}^{int} is purely quantum mechanical, depending on the exchange-correlation part of electron-electron interaction. Typically, V_C^{int} is associated with ionic-type interactions, while V_{XC}^{int} relates to covalent-type interactions.

Magnetically induced current densities were calculated using the AIMAll program[26] at the PBE0-D3/def2-TZVP level, with the external magnetic field aligned along the z-axis, orthogonal to the molecular plane. In our analysis, diatropic (aromatic) and paratropic (antiaromatic) ring currents circulate clockwise and counterclockwise, respectively. Visualization of these currents was performed with Paraview 5.10.0 software.[27]



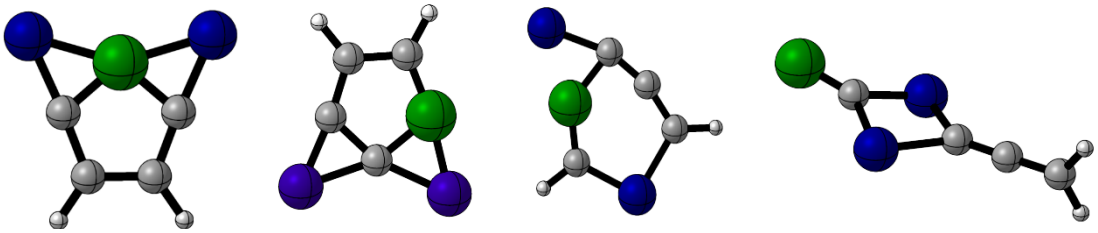
1a (C_{2v})	2a (C_s)	3a (C_s)	4a (C_s)
$^1A_1$	$^1A'$	$^1A'$	^1A
0.0	**7.9**	**10.9**	**60.5**
(0.0)	(8.5)	(12.0)	(58.0)

Figures S1. Global minimum and low-lying isomers of $C_4H_2Si_2B^-$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections. A number-letter label identifies structure to facilitates their connection with their Cartesian coordinates (at the end of the ESI).



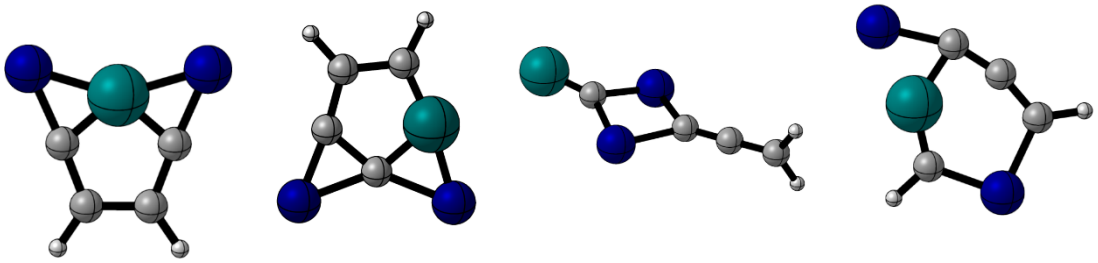
1b (C_{2v})	2b (C_s)	3b (C_s)	4b (C_s)
$^1A_1$	$^1A'$	$^1A'$	$^1A'$
0.0	**4.3**	**5.4**	**13.9**
(0.0)	(4.5)	(4.1)	(15.1)

Figures S2. Global minimum and low-lying isomers of $C_4H_2Si_2Al^-$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



1c (C_{2v})	2c (C_s)	3c (C_s)	4c (C_s)
$^1A_1$	$^1A'$	$^1A'$	$^1A'$
0.0	**4.6**	**6.6**	**15.2**
(0.0)	(1.99)	(6.1)	(10.5)

Figures S3. Global minimum and low-lying isomers of $C_4H_2Si_2Ga^-$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



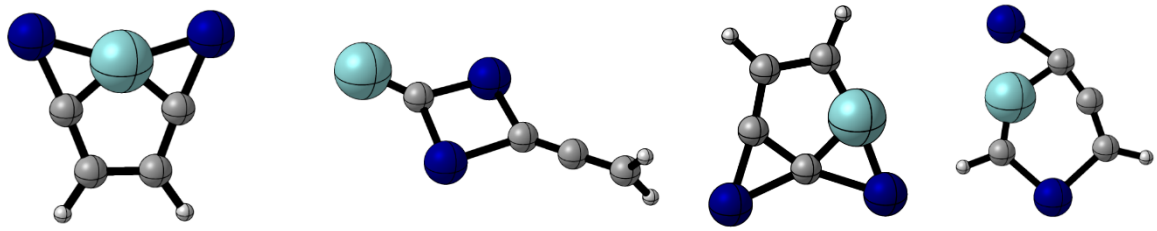
1d (C_{2v})
$^1A_1$
0.0
(0.0)

2d (C_s)
$^1A'$
9.1
(6.1)

3d (C_s)
$^1A'$
11.8
(8.5)

4d (C_s)
$^1A'$
14.2
(14.0)

Figures S4. Global minimum and low-lying isomers of $C_4H_2Si_2In^-$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



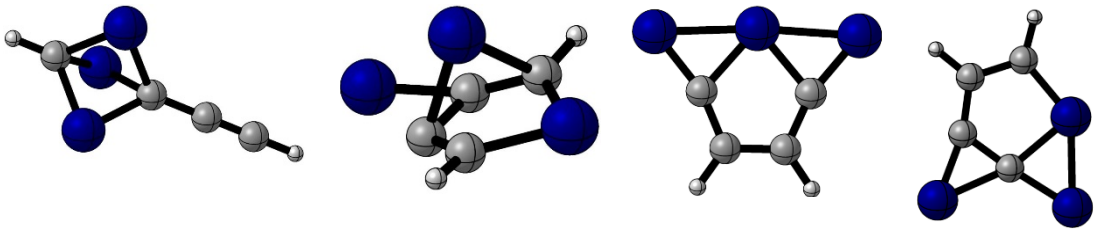
1e (C_{2v})
$^1A_1$
0.0
(0.0)

2e (C_s)
$^1A'$
14.5
(10.1)

3e (C_s)
$^1A'$
16.5
(11.6)

4e (C_s)
$^1A'$
24.4
(21.5)

Figures S5. Global minimum and low-lying isomers of $C_4H_2Si_2Tl^-$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



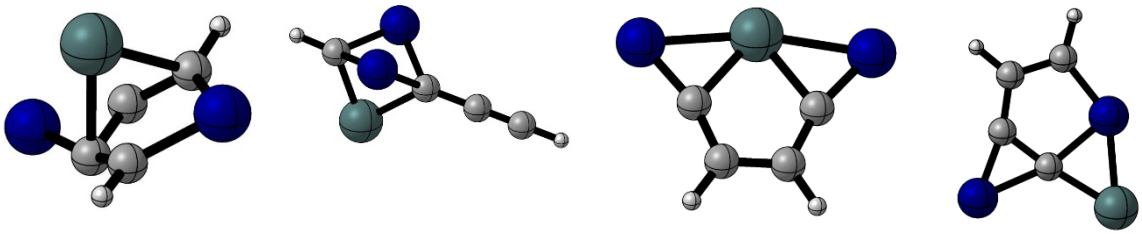
1f (C_{3v})
$^1A_1$
0.0
2.5

2f (C_s)
$^1A'$
0.9
0.5

3f (C_{2v})
$^1A_1$
1.7
0.0

4f (C_s)
$^1A'$
7.3
4.2

Figures S6. Global minimum and low-lying isomers of $C_4H_2Si_3$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



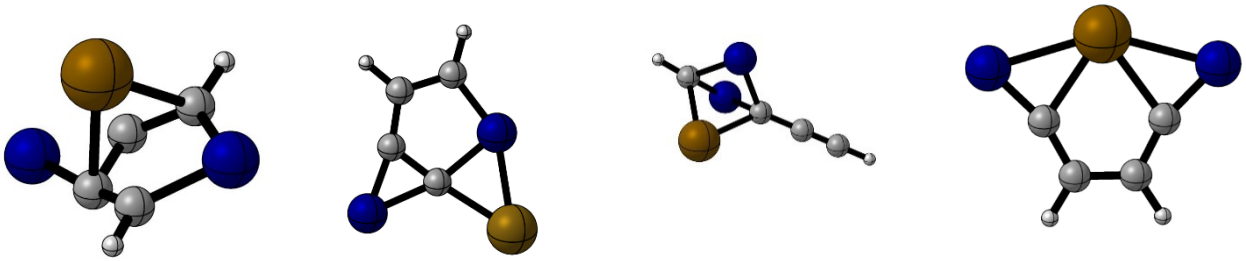
1g (C_s)
^{1}A'
0.0
0.0

2g (C_s)
^{1}A'
4.4
5.6

3g (C_{2v})
^{1}A$_1$
6.2
6.0

4g (C_s)
^{1}A'
9.6
3.9

Figures S7. Global minimum and low-lying isomers of $C_4H_2Si_2Ge$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



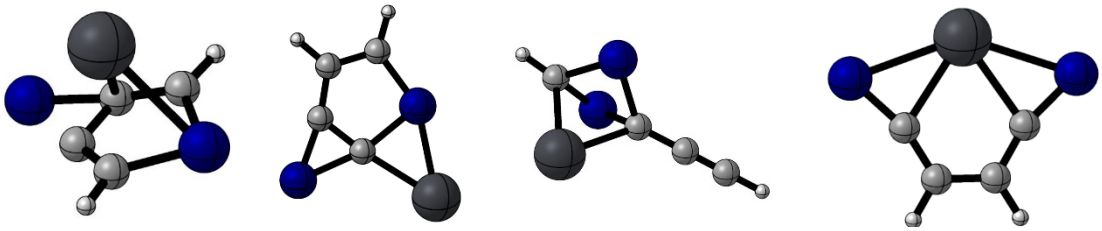
1h (C_s)
^{1}A'
0.0
0.0

2h (C_s)
^{1}A'
10.3
5.4

3h (C_s)
^{1}A'
10.9
12.2

4h (C_{2v})
^{1}A$_1$
13.8
13.0

Figures S8. Global minimum and low-lying isomers of $C_4H_2Si_2Sn$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



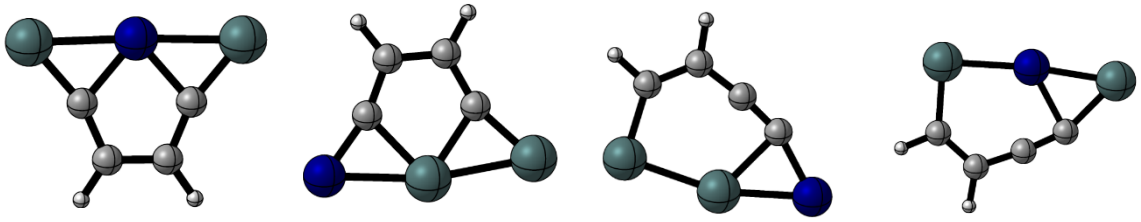
1i (C_s)
^{1}A'
0.0
0.0

2i (C_s)
^{1}A'
9.8
5.6

3i (C_s)
^{1}A'
14.2
14.9

4i (C_{2v})
^{1}A$_1$
15.6
14.7

Figures S9. Global minimum and low-lying isomers of $C_4H_2Si_2Pb$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels including zero-point energy (ZPE) corrections. A number-letter label identifies structure to facilitates their connection with their Cartesian coordinates (at the end of the ESI).



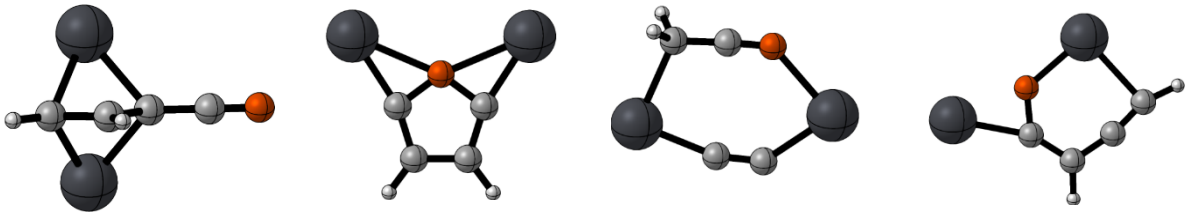
1j (C_{2v})
$^1A_1$
0.0
0.0

2j (C_s)
$^1A'$
0.6
3.2

3j (C_s)
$^1A'$
8.4
9.2

4j (C_s)
$^1A'$
10.7
9.9

Figures S10. Global minimum and low-lying isomers of $C_4H_2Ge_2Si$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



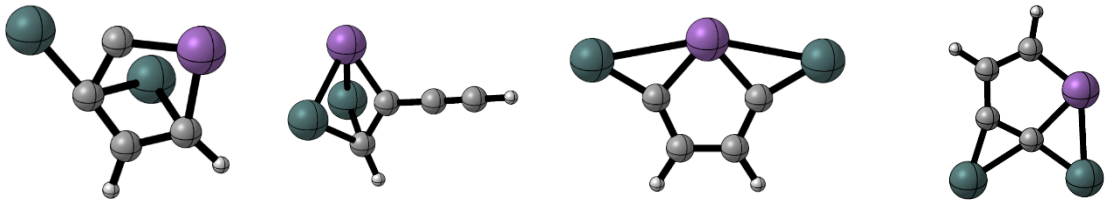
1k (C_s)
$^1A'$
0.0
0.0

2k (C_{2v})
$^1A'$
8.1
0.8

3k (C_s)
$^1A'$
8.6
8.3

4k (C_s)
$^1A'$
15.9
8.7

Figures S11. Global minimum and low-lying isomers of $C_4H_2Pb_2N^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



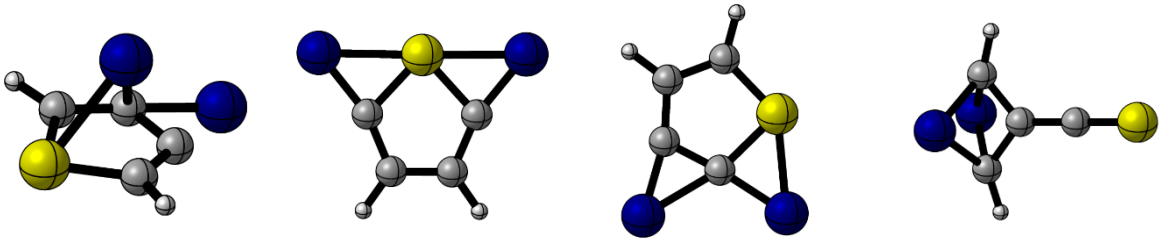
1m (C_s)
$^1A'$
0.0
0.0

2m (C_s) $^1A_1'$
14.8
11.8

3m (C_{2v})
$^1A'$
17.3
13.7

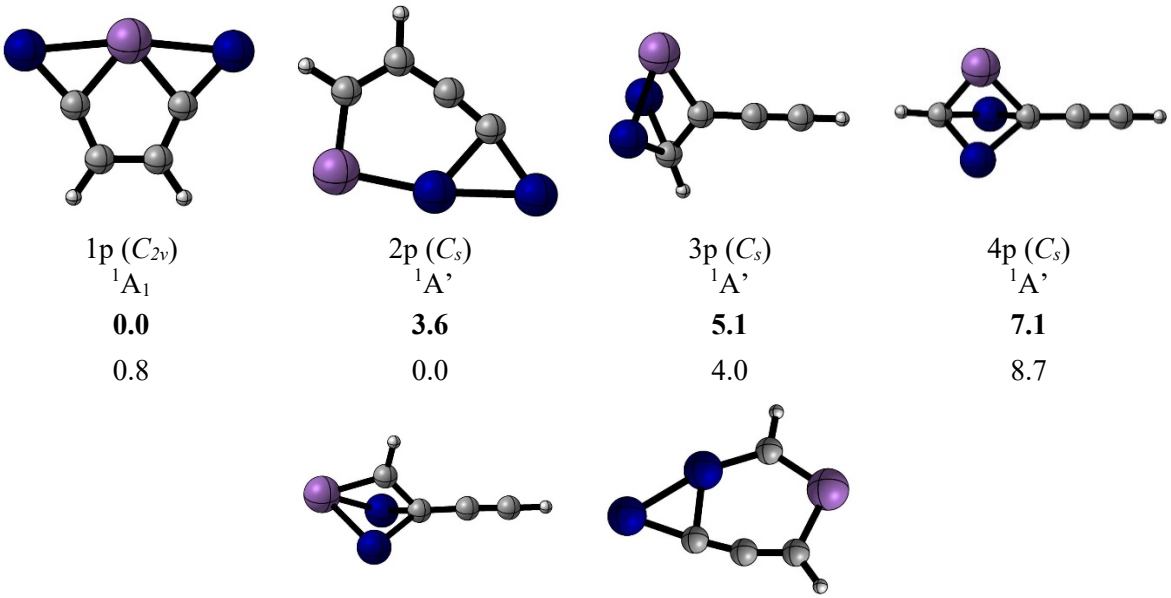
1m (C_s)
^1A
18.7
14.5

Figures S12. Global minimum and low-lying isomers of $C_4H_2Ge_2As^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



1n (C_s)	2n C_{2v})	3n (C_s)	4n (C_{2v})
^{1}A’	^{1}A$_1$	^{1}A’	^{1}A$_1$
0.0	**6.0**	**8.9**	**11.6**
0.0	4.4	7.1	13.4

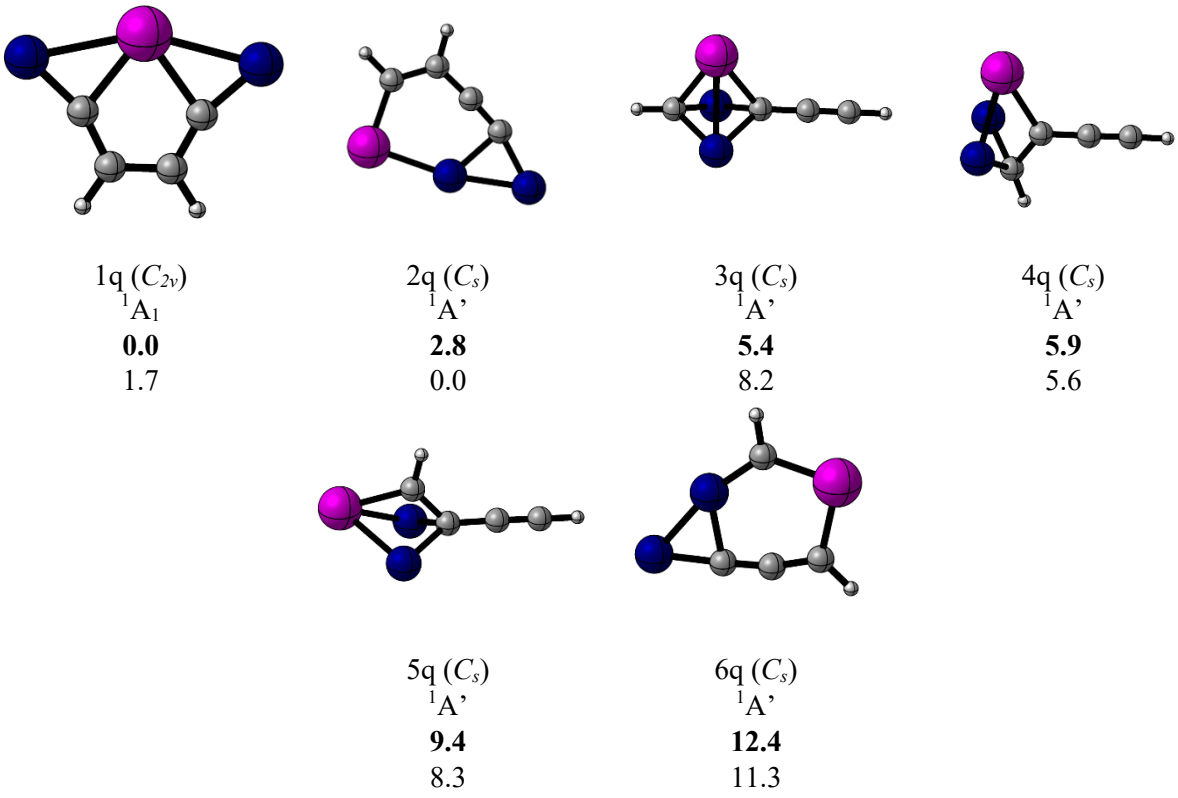
Figures S13. Global minimum and low-lying isomers of $C_4H_2Si_2P^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



1p (C_{2v})	2p (C_s)	3p (C_s)	4p (C_s)
^{1}A$_1$	^{1}A’	^{1}A’	^{1}A’
0.0	**3.6**	**5.1**	**7.1**
0.8	0.0	4.0	8.7

5p (C_s)	6p (C_s)
^{1}A’	^{1}A’
7.7	**11.8**
6.3	10.4

Figures S14. Global minimum and low-lying isomers of $C_4H_2Si_2As^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



1q (C_{2v})
$^1A_1$
0.0
1.7

2q (C_s)
$^1A'$
2.8
0.0

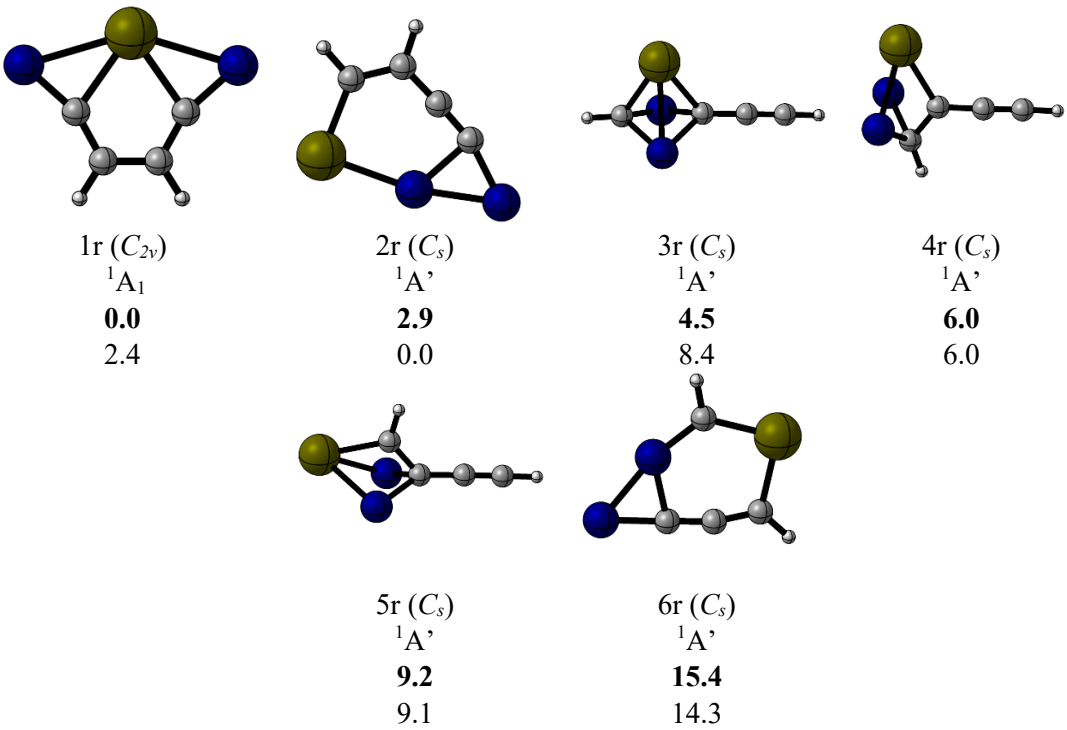
3q (C_s)
$^1A'$
5.4
8.2

4q (C_s)
$^1A'$
5.9
5.6

5q (C_s)
$^1A'$
9.4
8.3

6q (C_s)
$^1A'$
12.4
11.3

Figures S15. Global minimum and low-lying isomers of $C_4H_2Si_2Sb^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



1r (C_{2v})
$^1A_1$
0.0
2.4

2r (C_s)
$^1A'$
2.9
0.0

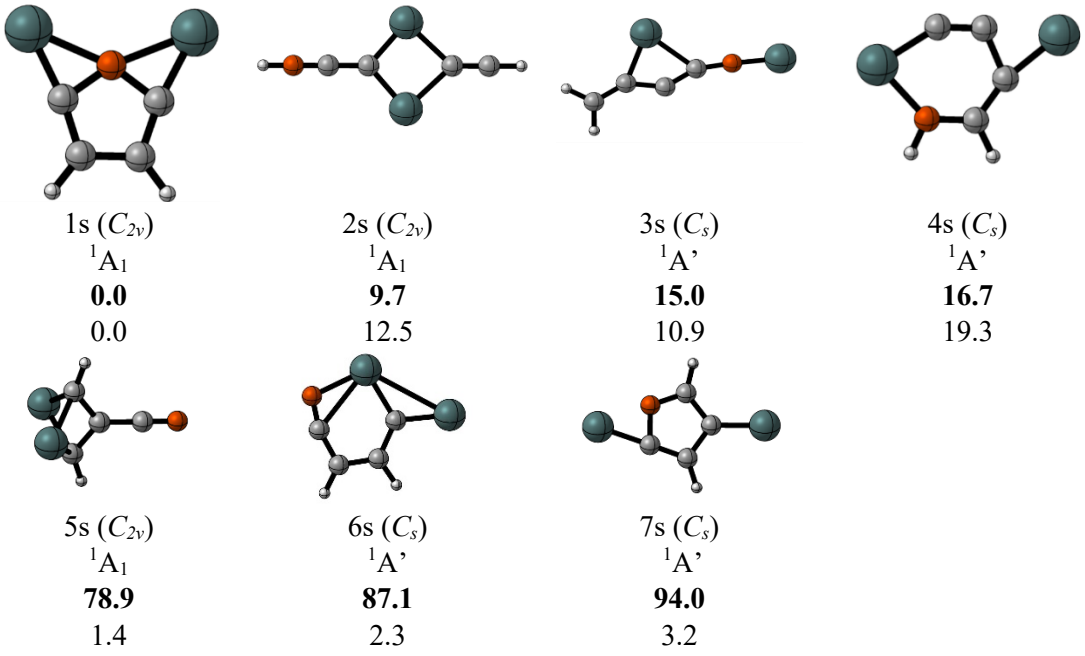
3r (C_s)
$^1A'$
4.5
8.4

4r (C_s)
$^1A'$
6.0
6.0

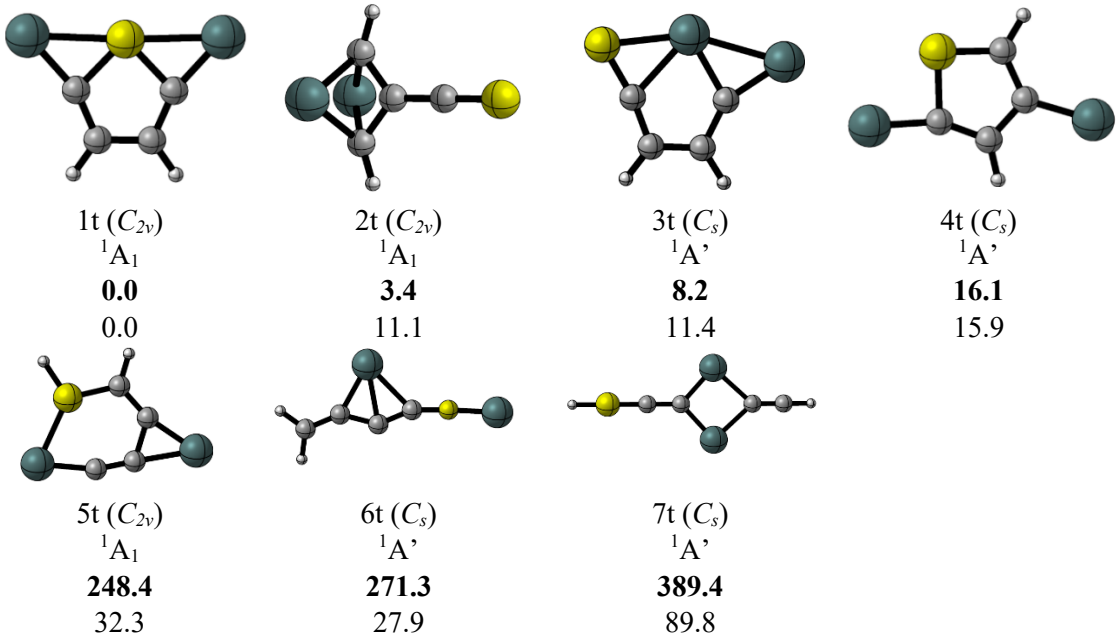
5r (C_s)
$^1A'$
9.2
9.1

6r (C_s)
$^1A'$
15.4
14.3

Figures S16. Global minimum and low-lying isomers of $C_4H_2Si_2Bi^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



Figures S17. Global minimum and low-lying isomers of $C_4H_2Ge_2N^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.



Figures S18. Global minimum and low-lying isomers of $C_4H_2Ge_2P^+$, their point group symmetries and spectroscopic states. Relative energies are shown in kcal/mol at DLPNO-CCSD(T)/CSB//PBE0-D3/def2-TZVP (**in bold**) and PBE0-D3/def2-TZVP (in parentheses) levels, including zero-point energy (ZPE) corrections.

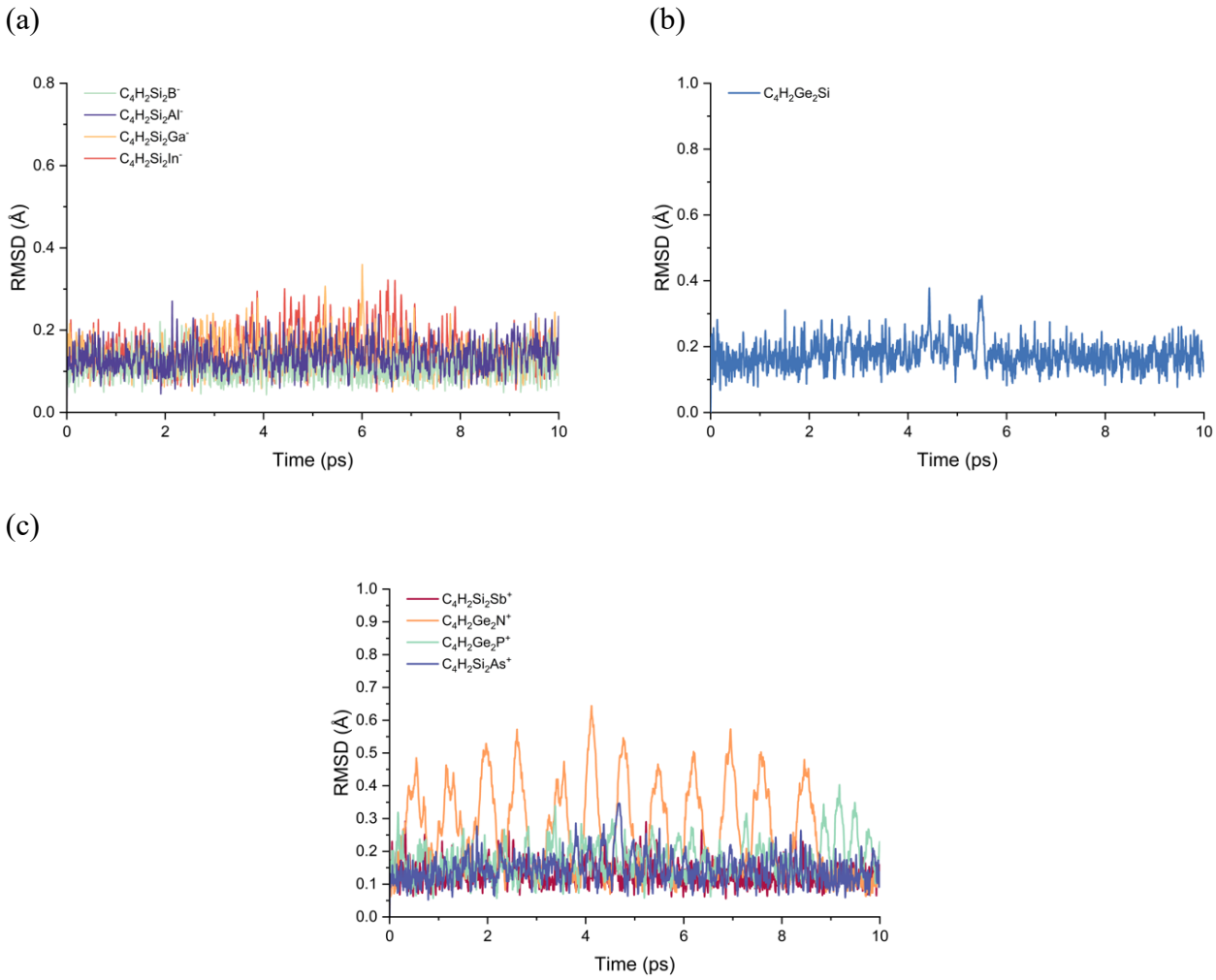


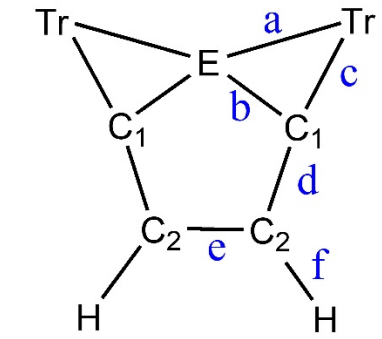
Figure S19. Born-Oppenheimer molecular dynamics (BO-MD) conducted at 450 K of minimum global of (a) $C_4H_3ETr_2^-$ (E = B/Al/Ga/In/Tl), (b) $C_4H_3Ge_2Si$ and (c) $C_4H_2ETr_2^+$ (E=As/Sb/Bi), $C_4H_2ETr_2^+$ (E=N/P).

Table S1. HOMO-LUMO energy gaps, singlet-triplet energy differences, smallest vibrational frequencies and T_1-diagnostics for the global minimum of $C_4H_3E\,Tr_2^-$ (E = B/Al/Ga/In/Tl), $C_4H_3Ge_2Si$, $C_4H_2E\,Tr_2^+$ (E=As/Sb/Bi), $C_4H_2ETr_2^+$ (E=N/P).

System	ΔE_{H-L} (eV)	ΔE_{S-T} (kcal/mol)	ν_{min} (cm^{-1})	T_1 Diagnostic
$C_4H_2Si_2B^-$	3.7	42.8	206	0.015
$C_4H_2Si_2Al^-$	2.8	22.9	121	0.017
$C_4H_2Si_2Ga^-$	2.8	23.8	103	0.015
$C_4H_2Si_2In^-$	2.9	25.5	85	0.016
$C_4H_2Si_2Tl^-$	3.3	27.6	75	0.016
$C_4H_2Ge_2Si$	4.1	46.3	98	0.014
$C_4H_2Ge_2N^+$	4.5	72.1	102	0.012
$C_4H_2Ge_2P^+$	4.6	63.9	78	0.013
$C_4H_2Si_2As^+$	4.8	63.3	82	0.012
$C_4H_2Si_2Sb^+$	4.2	36.3	78	0.013
$C_4H_2Si_2Bi^+$	3.8	34.7	78	0.013

Table S2. Natural charges (q, in |e|), Wiberg bond indices (WBI) and bond distances (r, in Å) of minimum global (a) $C_4H_3E\,Tr_2^-$ (E = B/Al/Ga/In/Tl), (b) $C_4H_3Ge_2Si$, and (c) $C_4H_2ETr_2^+$ (E=As/Sb/Bi, Tr=Si), $C_4H_2ETr_2^+$ (E=N/P, Tr=Ge) at PBE0-D3/def2-TZVP level.

(a)



q

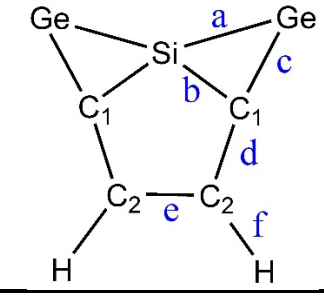
	E	Tr	C1	C2	H
B	-0.39	+0.57	-0.80	-0.26	+0.19
Al	+0.54	+0.38	-1.04	-0.28	+0.18
Ga	+0.35	+0.43	-0.99	-0.29	+0.18
In	+0.27	+0.43	-0.95	-0.31	+0.18
Tl	+0.28	+0.39	-0.90	-0.32	+0.19

r

WBI

a	b	c	d	e	f
1.99	1.58	1.73	1.42	1.38	1.09
0.78	1.02	1.23	1.26	1.57	0.91
2.45	2.08	1.72	1.42	1.37	1.09
0.78	0.53	1.54	1.26	1.59	0.90
2.44	2.13	1.72	1.41	1.37	1.09
0.74	0.55	1.51	1.28	1.57	0.89
2.73	2.56	1.69	1.40	1.37	1.09
0.49	0.41	1.76	1.30	1.55	0.89
2.88	2.77	1.68	1.39	1.37	1.09
0.37	0.33	1.89	1.32	1.54	0.89

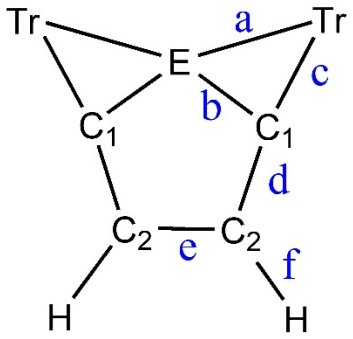
(b)



	q				
	Si	Ge	C1	C2	H
Si	+0.44	+0.76	-0.96	-0.25	+0.23

	r					
	WBI					
	a	b	c	d	e	f
	2.43	1.91	1.83	1.41	1.37	1.09
	0.68	0.91	1.22	1.28	1.56	0.89

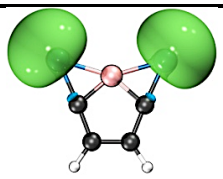
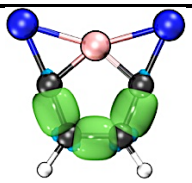
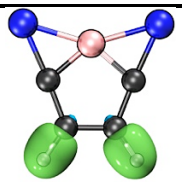
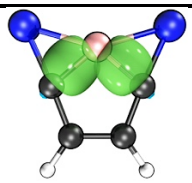
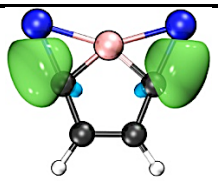
(c)



	q				
	E	Tr	C1	C2	H
As	+0.44	+1.13	-0.92	-0.20	+0.27
Sb	+0.69	+1.07	-0.95	-0.22	+0.27
Bi	+0.73	+1.02	-0.92	-0.24	+0.27
	Tr	Si	C1	C2	H
N	-0.77	+1.26	-0.44	-0.21	+0.27
P	+0.34	+1.17	-0.90	-0.20	+0.27

	r					
	WBI					
	a	b	c	d	e	f
	2.47	1.98	1.75	1.40	1.37	1.09
	0.46	1.03	1.03	1.34	1.51	0.88
	2.66	2.22	1.73	1.39	1.37	1.09
	0.47	0.92	1.15	1.36	1.49	0.87
	2.75	2.36	1.72	1.39	1.37	1.09
	0.47	0.85	1.23	1.38	1.47	0.87
	2.12	1.40	1.86	1.40	1.38	1.08
	0.25	1.20	0.83	1.34	1.53	0.90
	2.47	1.81	1.86	1.40	1.37	1.08
	0.41	1.16	0.94	1.32	1.52	0.88

[a]The sums of Pyykkö´s single-bond radii for the B-Si, Al-Si, Ga-Si, In-Si, Tl-Si, Si-Ge, As-Si, Sb-Si, Bi-Si, N-Ge and P-Ge bond are 2.01, 2.42, 2.40, 2.58, 2.60, 2.37, 2.42, 2.61, 2.72, 1.92, and 2.32 Å.

	Si-Lone Pairs	σ-bonds			
					
	2 x 1c-2e	3 x 2c-2e C-C	2 x 2c-2e C-H	2 x 2c-2e C-E	2 x 2c-2e C-Si or Ge
E = B	1.94 |e|	1.99 |e|	1.98 |e|	1.82 |e|	1.96 |e|
E = Al	1.88 |e|	1.99 |e|	1.97 |e|	1.63 |e|	1.97 |e|
E = Ga	1.90 |e|	1.99 |e|	1.97 |e|	1.61 |e|	1.97 |e|

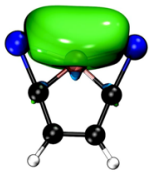
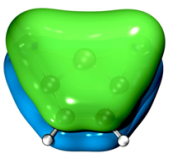
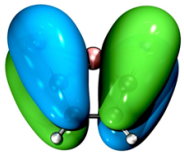
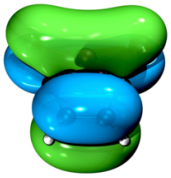
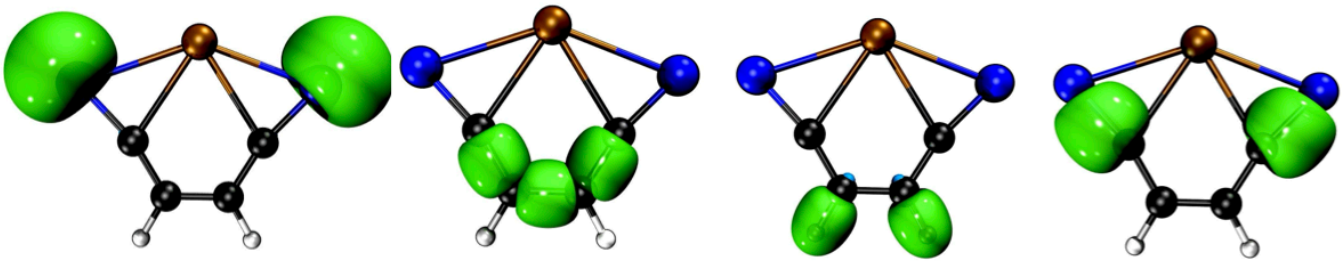
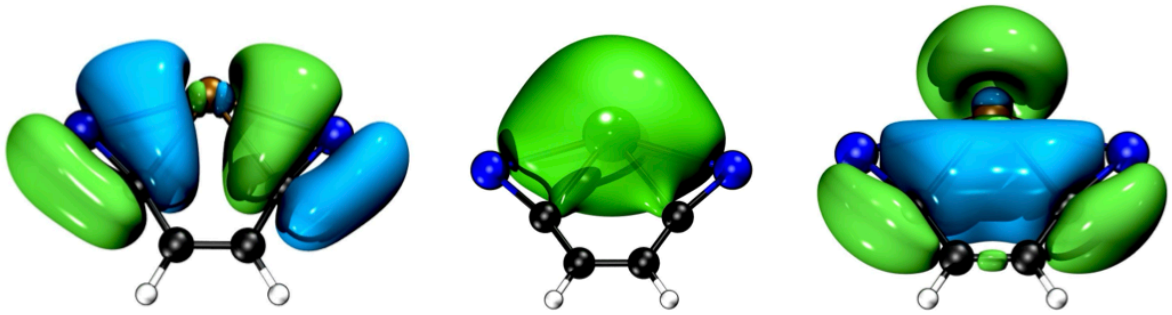
	σ-bonds	π-bonds	
			 
	1 x 3c-2e	3 x 7c-2e	
E = B	1.94 |e|	2.00 |e|	
E = Al	1.92 |e|	2.00 |e|	
E = Ga	1.91 |e|	2.00 |e|	

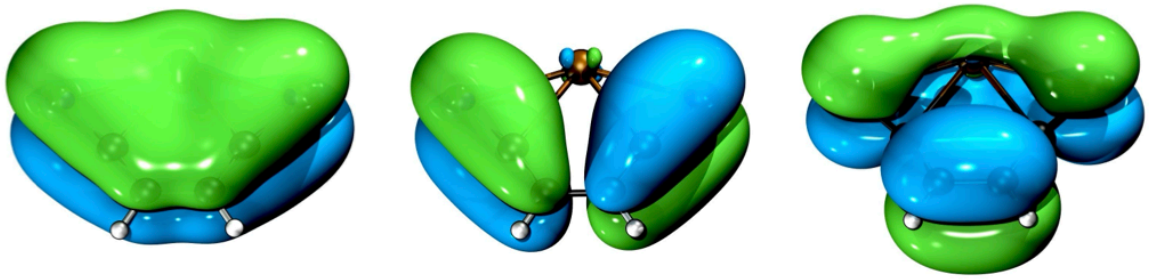
Figure S20. The adaptive natural density partitioning (AdNDP) bonding pattern of minimum global of $C_4H_3ETr_2^-$ (E = B/Al/Ga) at the PBE0-D3/def2-TZVP level.



	2 × 1c-2e Si-LPs	3 × 2c-2e C-C σ-bonds	2 × 2c-2e C-H σ-bonds	2 × 2c-2e C-Si σ-bonds
$C_4H_2Si_2In^-$	ON = 1.90 |e|	ON = 1.99 |e|	ON = 1.96 |e|	ON = 1.98 |e|
$C_4H_2Si_2Tl^-$	ON = 1.91 |e|	ON = 1.99 |e|	ON = 1.96 |e|	ON = 1.99 |e|



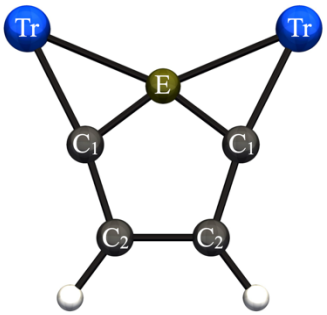
	1 × 5c-2e σ-bond	1 × 5c-2e σ-bond	1 × 7c-2e σ-bond
$C_4H_2Si_2In^-$	ON = 1.97 |e|	ON = 2.00 |e|	ON = 1.96 |e|
$C_4H_2Si_2Tl^-$	ON = 1.97 |e|	ON = 2.00 |e|	ON = 1.97 |e|



	3 × 7c-2e π-bond
$C_4H_2Si_2In^-$	ON = 2.00 |e|
$C_4H_2Si_2Tl^-$	ON = 2.00 |e|

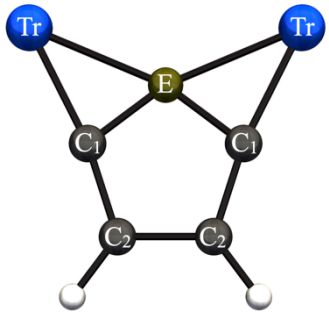
Figure S21. The adaptive natural density partitioning (AdNDP) bonding pattern of minimum global of $C_4H_2Si_2In^-$ and $C_4H_2Si_2Tl^-$.

Table S3. QTAIM atomic charges for $C_4H_2ETr_2^n$ (E = B-Tl with Tr = Si and n = –1; E = Si with Tr = Ge and n = 0; E = N-P with Tr = Ge and n = +1; E = As-Bi with Tr = Si and n = +1) at PBE0-D3/def2-TZVP level.



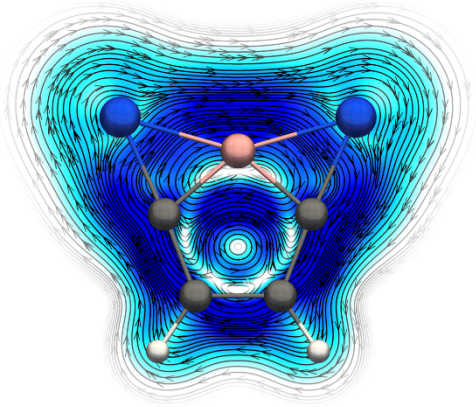
	B	Al	Ga	In	Tl	Si	N	P	As	Sb	Bi
E	0.49	1.23	0.29	0.21	0.16	1.04	–1.29	0.78	0.38	0.66	0.66
Tr	1.00	0.72	0.85	0.85	0.83	0.71	1.16	1.06	1.36	1.30	1.26
C1	–1.69	–1.81	–1.47	–1.44	–1.40	–1.29	–0.16	–1.11	–1.23	–1.30	–1.27
C2	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.04	0.05	0.05	0.05
H	0.00	0.00	0.00	0.00	0.00	0.01	0.13	0.12	0.13	0.12	0.12

Table S4. Energy components of IQA and delocalization indices (δ) between atom pairs for $C_4H_2ETr_2^n$ (E = B-Tl with Tr = Si and n = –1; E = Si with Tr = Ge and n = 0; E = N-P with Tr = Ge and n = +1; E = As-Bi with Tr = Si and n = +1). ΔE_{IQA} is the total integration error in IQA energies, V_{IQA}^{int}, V_C^{int}, and V_{XC}^{int} are interatomic IQA interaction energy, Coulomb energy component, and exchange-correlation energy component of the interaction energy, respectively, in kcal/mol.



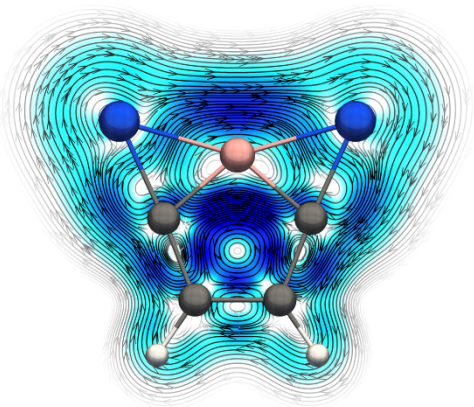
	B	Al	Ga	In	Tl	Si	N	P	As	Sb	Bi
ΔE_{IQA}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
V_{IQA}^{int}(E-Tr)	94.6	175.2	41.3	27.9	10.9	116.1	–343.0	114.6	66.6	113.3	98.5
V_C^{int}(E-Tr)	154.7	217.1	97.2	69.4	45.7	174.4	–287.4	161.8	112.4	155.6	139.7
V_{XC}^{int}(E-Tr)	–60.1	–41.9	–55.9	–41.5	–34.8	–58.3	–55.6	–47.1	–45.8	–42.4	–41.2
V_{IQA}^{int}(E-C_1)	–481.4	–584.8	–244.2	–163.7	–115.2	–521.5	–290.7	–461.8	–285.9	–307.8	–266.1
V_C^{int}(E-C_1)	–331.3	–518.3	–144.8	–99.2	–62.9	–411.8	–72.0	–290.0	–122.8	–176.6	–150.8
V_{XC}^{int}(E-C_1)	–150.1	–66.5	–99.4	–64.5	–52.3	–109.6	–218.8	–170.9	–163.1	–131.2	–115.4
V_{IQA}^{int}(C_1-Tr)	–834.3	–762.8	–713.8	–723.0	–715.4	–477.6	–209.0	–473.4	–707.3	–727.9	–713.1
V_C^{int}(C_1-Tr)	–682.9	–577.6	–549.8	–544.1	–529.6	–293.0	–77.2	–318.0	–581.3	–590.7	–571.5
V_{XC}^{int}(C_1-Tr)	–151.4	–185.2	–164.0	–178.9	–185.8	–184.5	–131.8	–155.4	–126.0	–137.2	–141.6
V_{IQA}^{int}(C_1-C_2)	–222.2	–225.3	–226.7	–229.7	–230.5	–231.0	–213.5	–239.9	–246.4	–248.4	–249.9
V_C^{int}(C_1-C_2)	19.9	18.6	20.0	21.3	23.7	12.7	28.9	6.3	4.6	5.5	8.0
V_{XC}^{int}(C_1-C_2)	–242.1	–243.9	–246.7	–251.0	–254.1	–243.7	–242.4	–246.2	–251.0	–253.9	–257.9
δ(E-Tr)	0.5	0.5	0.6	0.4	0.4	0.6	0.5	0.5	0.5	0.5	0.5
δ(E-C_1)	0.9	0.5	0.8	0.6	0.6	0.8	1.2	1.2	1.2	1.1	1.0
δ(C_1-Tr)	1.2	1.5	1.3	1.4	1.5	1.4	0.9	1.1	0.9	1.0	1.1
δ(C_1-C_2)	1.3	1.3	1.3	1.3	1.4	1.3	1.3	1.3	1.3	1.4	1.4

$C_4H_2Si_2B^-$-Total



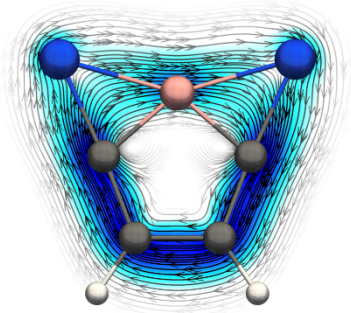
8.0 nA/T

$C_4H_2Si_2B^-$-σ



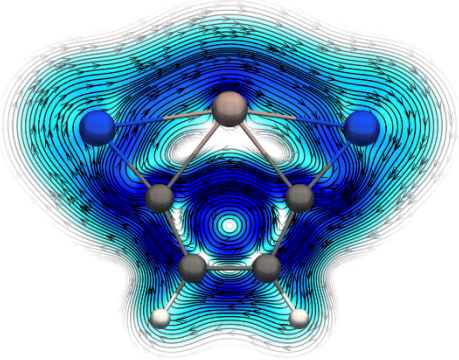
0.0 nA/T

$C_4H_2Si_2B^-$-π



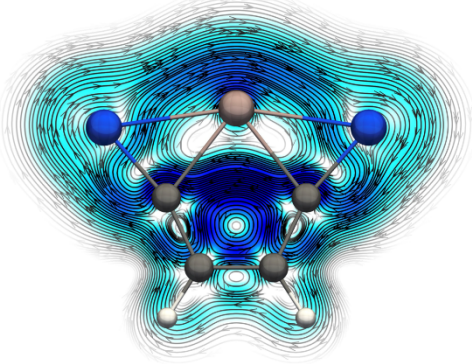
8.0 nA/T

$C_4H_2Si_2Al^-$-Total



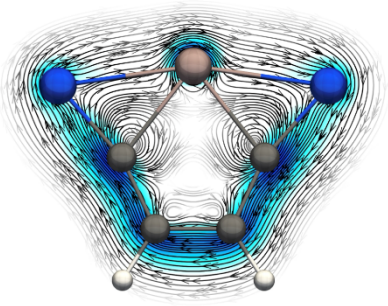
5.2 nA/T

$C_4H_2Si_2Al^-$-σ



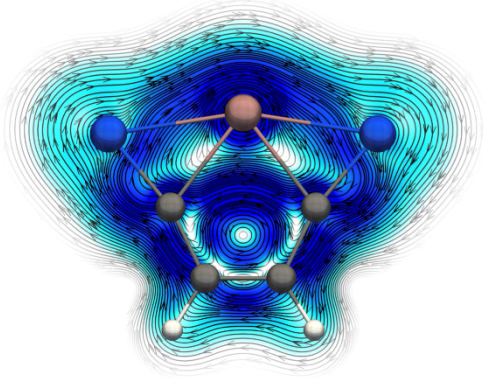
0.0 nA/T

$C_4H_2Si_2Al^-$-π



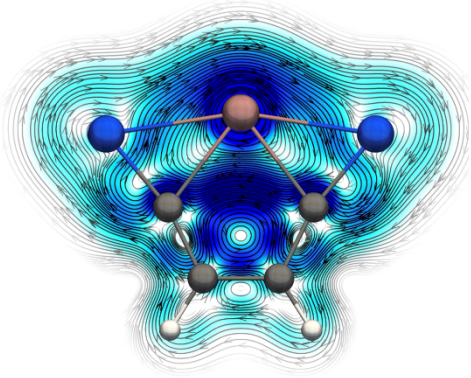
5.2 nA/T

$C_4H_2Si_2Ga^-$-Total



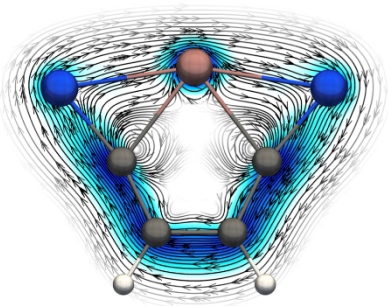
6.2 nA/T

$C_4H_2Si_2Ga^-$-σ



0.2 nA/T

$C_4H_2Si_2Ga^-$-π



6.0 nA/T

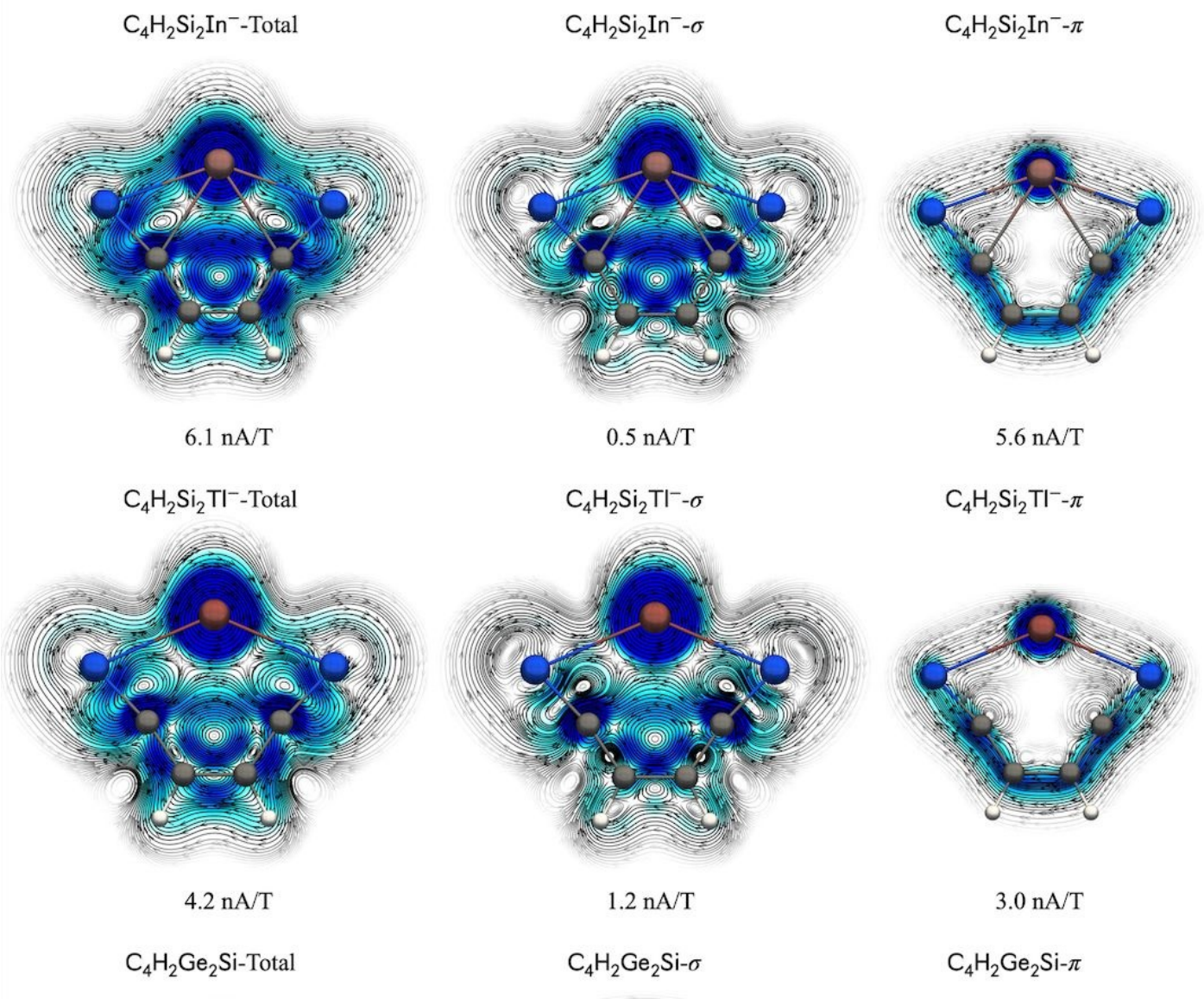


Figure S22. Vector maps of current density located 0.5 Å above the molecular plane for $C_4H_2Si_2E^-$ (E = B, Al, Ga, In and Tl). Corresponding current strengths in nA/T are also provided at the PBE0-D3/def2-TZVP level.

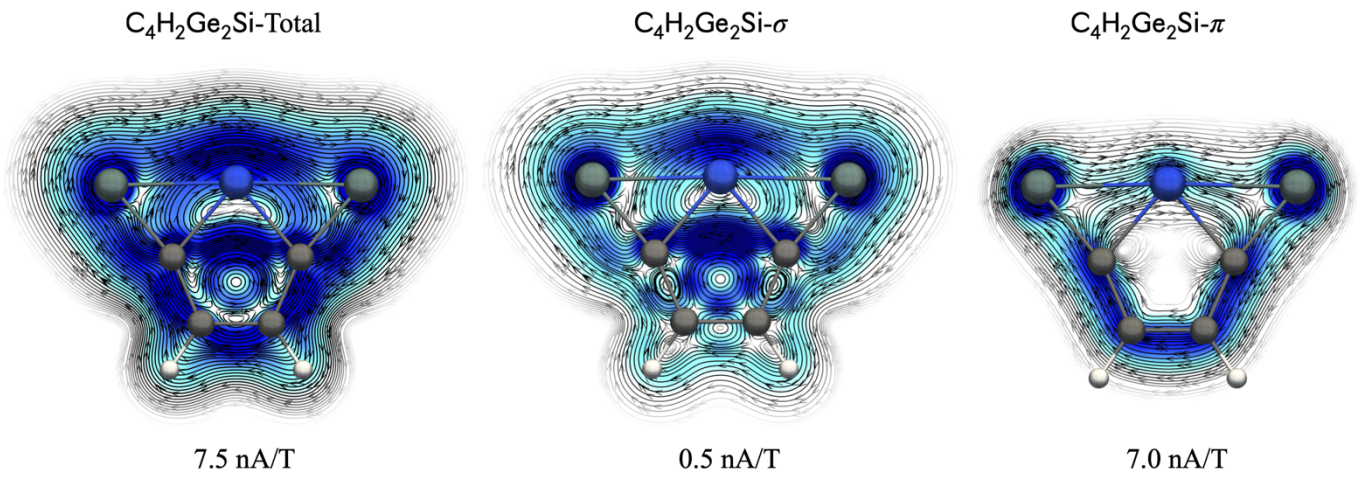


Figure S23. Vector maps of current density located 0.5 Å above the molecular plane for $C_4H_2Ge_2Si$. Corresponding current strengths in nA/T are also provided at the PBE0-D3/def2-TZVP level.

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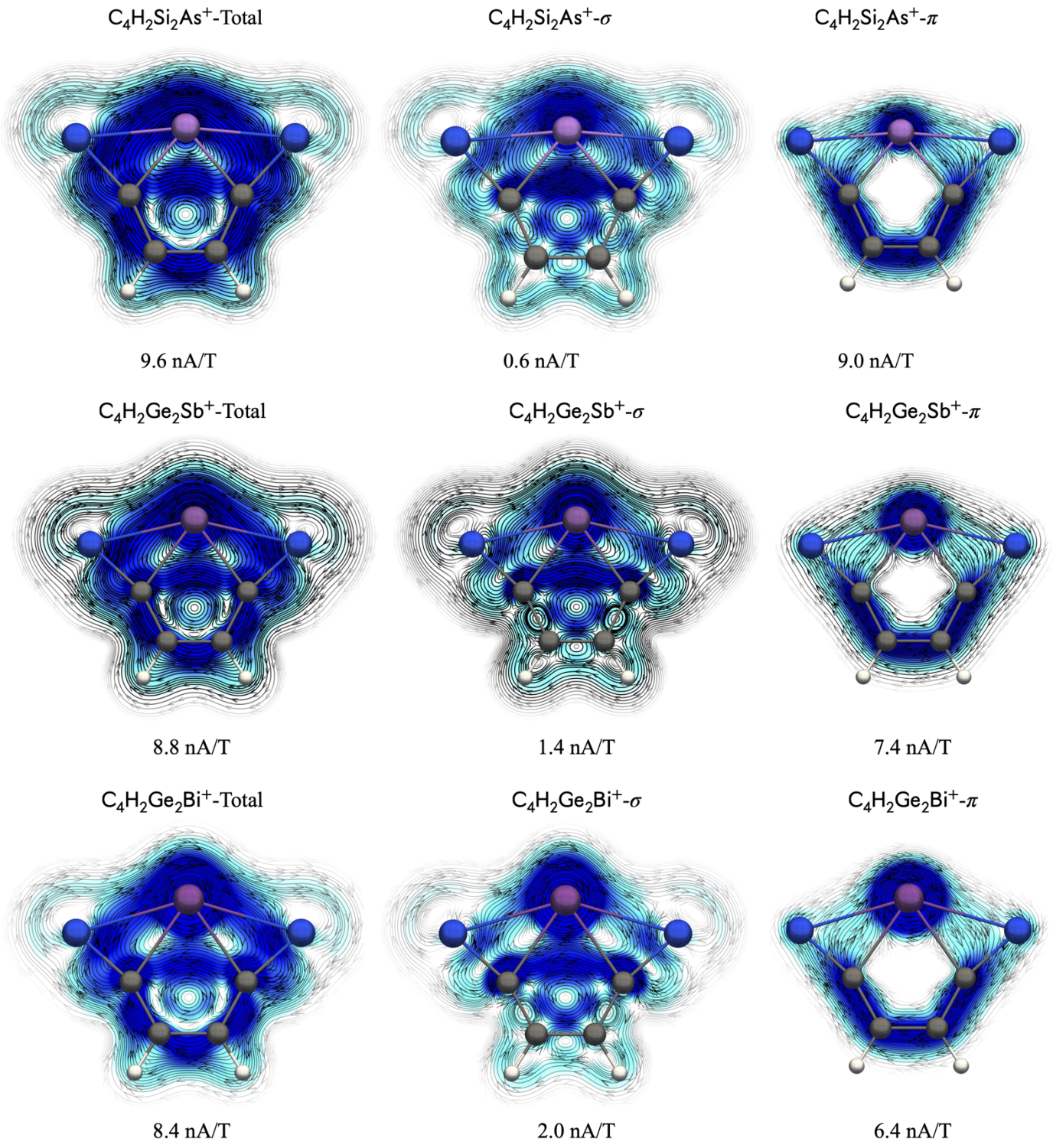

Figure S24. Vector maps of current density located 0.5 Å above the molecular plane for $C_4H_2Si_2E^+$ (E = As, Sb and Bi). Corresponding current strengths in nA/T are also provided at the PBE0-D3/def2-TZVP level

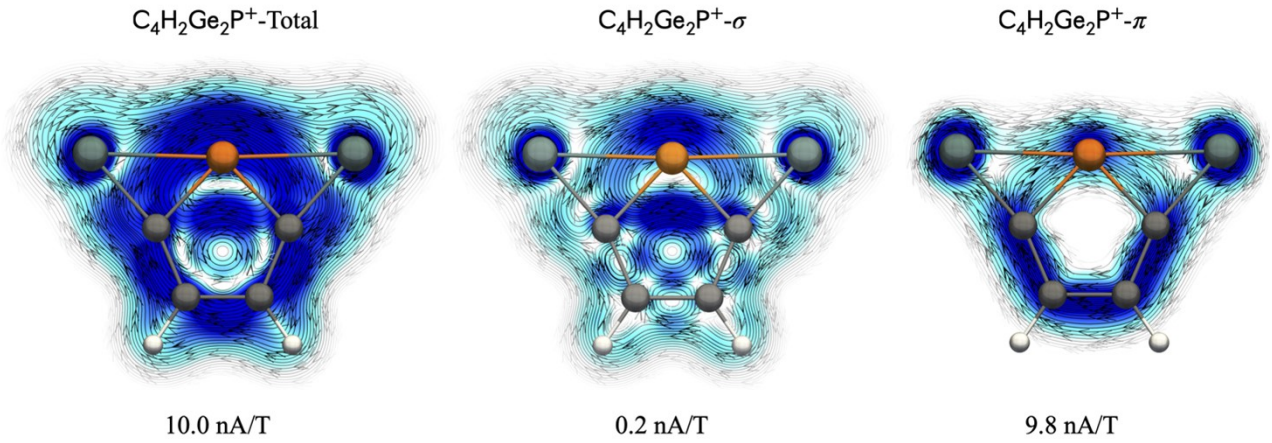

Figure S25. Vector maps of current density located 0.5 Å above the molecular plane for $C_4H_2Ge_2P^+$. Corresponding current strengths in nA/T are also provided at the PBE0-D3/def2-TZVP level.

Cartesian Coordinates

Cartesian Coordinates of $C_4H_3Tr_2E^-$ (E = B/Al/Ga/In/Tl), $C_4H_3Ge_2Si$, $C_4H_3Tr_2E^+$ (E=As/Sb/Bi), $C_4H_3Tr_2E^+$ (E=N/P) cluster calculated at the PBE0-D3/def2-TZVP level.

1a

C	0.000000000	1.197523000	-0.491248000
H	0.000000000	-1.304556000	-2.716337000
C	0.000000000	-1.197523000	-0.491248000
C	0.000000000	0.688410000	-1.816278000
B	0.000000000	0.000000000	0.536088000
Si	0.000000000	1.914360000	1.087234000
H	0.000000000	1.304556000	-2.716337000
C	0.000000000	-0.688410000	-1.816278000
Si	0.000000000	-1.914360000	1.087234000

2a

C	-0.791906000	-1.949674000	0.000000000
H	1.252489000	-2.768177000	0.000000000
C	0.585382000	-1.906039000	0.000000000
C	0.000000000	0.459305000	0.000000000
B	-1.312011000	-0.521328000	0.000000000
C	1.050699000	-0.572393000	0.000000000
Si	-1.690967000	1.289134000	0.000000000
H	-1.343593000	-2.887547000	0.000000000
Si	1.804260000	1.001949000	0.000000000

3a

Si	-1.884517000	-1.215252000	0.000000000
Si	1.704925000	1.927989000	0.000000000
H	0.136757000	-2.966137000	0.000000000
C	-1.406627000	0.526387000	0.000000000
C	-0.101274000	-1.905834000	0.000000000
B	0.000000000	0.963880000	0.000000000
C	1.437245000	0.168134000	0.000000000
C	0.833606000	-0.973188000	0.000000000
H	-2.200177000	1.275427000	0.000000000

4a

H	3.716929000	-0.002292000	1.299740000
B	-3.210359000	-0.002478000	0.626825000
C	3.326067000	-0.001320000	0.287739000
Si	-0.623964000	1.322473000	-0.229457000
C	2.026540000	-0.000714000	0.054145000
C	-1.811800000	0.001533000	0.221722000
H	4.040097000	-0.000883000	-0.529035000
C	0.758038000	-0.000060000	-0.141715000
Si	-0.625915000	-1.321121000	-0.230270000

1b

C	0.000000000	1.283308000	-0.559388000
H	0.000000000	-1.271648000	-2.763005000
C	0.000000000	-1.283308000	-0.559388000
C	0.000000000	0.682720000	-1.840459000
Al	0.000000000	0.000000000	1.078422000
Si	0.000000000	2.425356000	0.725167000
H	0.000000000	1.271648000	-2.763005000
C	0.000000000	-0.682720000	-1.840459000
Si	0.000000000	-2.425356000	0.725167000

2b

Si	2.168525000	-1.159366000	0.000000000
Si	-2.386894000	1.356108000	0.000000000
H	0.298985000	-3.032965000	0.000000000
C	1.771872000	0.592745000	0.000000000
C	0.414458000	-1.948965000	0.000000000
Al	0.000000000	1.182174000	0.000000000
C	-1.507871000	-0.203523000	0.000000000
C	-0.655355000	-1.168301000	0.000000000
H	2.619555000	1.278581000	0.000000000

3b

C	-0.141038000	-2.281566000	0.000000000
H	-2.294817000	-2.007471000	0.000000000
C	-1.299828000	-1.549851000	0.000000000
C	0.000000000	0.644261000	0.000000000
Al	1.370999000	-1.061379000	0.000000000
C	-1.205931000	-0.135402000	0.000000000
Si	1.723290000	1.237947000	0.000000000
H	-0.211190000	-3.369373000	0.000000000
Si	-1.683018000	1.555634000	0.000000000

4b

H	0.968576000	4.200073000	0.000000000
Al	1.061894000	-3.038857000	0.000000000
C	-0.033990000	3.784051000	0.000000000
Si	-0.401535000	-0.212069000	1.296976000
C	-0.237764000	2.476883000	0.000000000
C	0.229239000	-1.339406000	0.000000000
H	-0.865918000	4.481069000	0.000000000
C	-0.401535000	1.205462000	0.000000000
Si	-0.401535000	-0.212069000	-1.296976000

1c

C	0.000000000	1.299447000	-0.818277000
H	0.000000000	-1.267121000	-3.012147000
C	0.000000000	-1.299447000	-0.818277000
C	0.000000000	0.683292000	-2.085738000
Ga	0.000000000	0.000000000	0.871391000
Si	0.000000000	2.405388000	0.494977000
H	0.000000000	1.267121000	-3.012147000
C	0.000000000	-0.683292000	-2.085738000
Si	0.000000000	-2.405388000	0.494977000

2c

C	1.106635000	-1.755200000	0.000000000
H	3.037742000	-0.778363000	0.000000000
C	1.947867000	-0.673733000	0.000000000
C	0.000000000	0.966319000	0.000000000
Ga	-0.760358000	-1.191974000	0.000000000
C	1.387328000	0.626432000	0.000000000
Si	-1.817723000	0.865561000	0.000000000
H	1.528787000	-2.759850000	0.000000000
Si	1.271550000	2.384902000	0.000000000

3c

Si	2.162267000	-1.438198000	0.000000000
Si	-2.367670000	1.050390000	0.000000000
H	0.320559000	-3.324370000	0.000000000
C	1.744215000	0.310189000	0.000000000
C	0.423561000	-2.239248000	0.000000000
Ga	0.000000000	1.007848000	0.000000000
C	-1.516502000	-0.519860000	0.000000000
C	-0.654670000	-1.468898000	0.000000000
H	2.575448000	1.017299000	0.000000000

4c

H	-2.829122000	-4.029188000	0.000000000
Ga	0.348752000	2.539690000	0.000000000
C	-1.745726000	-4.098199000	0.000000000
Si	0.348752000	-0.675360000	1.298794000
C	-0.985740000	-3.015100000	0.000000000
C	0.268898000	0.609972000	0.000000000
H	-1.307511000	-5.091237000	0.000000000
C	-0.277387000	-1.946653000	0.000000000
Si	0.348752000	-0.675360000	-1.298794000

1d

2d

C	0.000000000	1.407539000	-1.164102000
H	0.000000000	-1.224486000	-3.315467000
C	0.000000000	-1.407539000	-1.164102000
C	0.000000000	0.682358000	-2.363799000
In	0.000000000	0.000000000	0.967841000
Si	0.000000000	2.571387000	0.055056000
H	0.000000000	1.224486000	-3.315467000
C	0.000000000	-0.682358000	-2.363799000
Si	0.000000000	-2.571387000	0.055056000

C	1.614471000	1.279072000	0.000000000
H	3.290012000	-0.077319000	0.000000000
C	2.200700000	0.044747000	0.000000000
C	0.000000000	-1.251805000	0.000000000
In	-0.551452000	1.208011000	0.000000000
C	1.413534000	-1.137345000	0.000000000
Si	-1.766882000	-1.056887000	0.000000000
H	2.273581000	2.150138000	0.000000000
Si	1.058692000	-2.862640000	0.000000000

3d

H	-2.880496000	-4.575048000	0.000000000
In	0.288241000	2.197972000	0.000000000
C	-1.796794000	-4.641929000	0.000000000
Si	0.288241000	-1.207866000	1.296419000
C	-1.038260000	-3.557249000	0.000000000
C	0.173544000	0.075421000	0.000000000
H	-1.357489000	-5.634651000	0.000000000
C	-0.331254000	-2.488019000	0.000000000
Si	0.288241000	-1.207866000	-1.296419000

4d

Si	2.230858000	-1.667319000	0.000000000
Si	-2.538829000	0.624568000	0.000000000
H	0.414039000	-3.546640000	0.000000000
C	1.872697000	0.092331000	0.000000000
C	0.490401000	-2.457929000	0.000000000
In	0.000000000	0.960894000	0.000000000
C	-1.548164000	-0.851845000	0.000000000
C	-0.620353000	-1.733757000	0.000000000
H	2.730065000	0.768565000	0.000000000

1e

C	0.000000000	1.470034000	-1.525170000
H	0.000000000	-1.199993000	-3.646010000
C	0.000000000	-1.470034000	-1.525170000
C	0.000000000	0.683920000	-2.680535000
Tl	0.000000000	0.000000000	0.824750000
Si	0.000000000	2.636721000	-0.323010000
H	0.000000000	1.199993000	-3.646010000
C	0.000000000	-0.683920000	-2.680535000
Si	0.000000000	-2.636721000	-0.323010000

2e

H	-0.447887000	-5.910663000	0.000000000
Tl	-0.531263000	1.635093000	0.000000000
C	0.558905000	-5.503664000	0.000000000
Si	0.953773000	-1.503265000	1.296077000
C	0.776086000	-4.197533000	0.000000000
C	0.276535000	-0.408932000	0.000000000
H	1.382731000	-6.210859000	0.000000000
C	0.953773000	-2.928139000	0.000000000
Si	0.953773000	-1.503265000	-1.296077000

3e

C	2.031014000	0.090524000	0.000000000
H	2.953704000	-1.853889000	0.000000000
C	2.022882000	-1.273696000	0.000000000
C	-0.515371000	-1.507976000	0.000000000
Tl	0.000000000	1.069948000	0.000000000
C	0.806108000	-2.009767000	0.000000000
Si	-2.048658000	-0.658042000	0.000000000
H	3.008779000	0.581388000	0.000000000
Si	-0.239220000	-3.426800000	0.000000000

4e

Si	2.240510000	-1.917642000	0.000000000
Si	-2.551792000	0.312083000	0.000000000
H	0.448526000	-3.803169000	0.000000000
C	1.890155000	-0.154739000	0.000000000
C	0.508775000	-2.712984000	0.000000000
Tl	0.000000000	0.766562000	0.000000000
C	-1.584391000	-1.175720000	0.000000000
C	-0.619686000	-2.013454000	0.000000000
H	2.740311000	0.530868000	0.000000000

1f

H	0.000000000	0.000000000	2.884849761
Si	-0.739758346	1.281299040	0.604999064
C	0.000000000	0.000000000	1.802517712
H	0.000000000	0.000000000	-4.306952337
Si	-0.739758346	-1.281299040	0.604999064
C	0.000000000	0.000000000	-3.242888377
Si	1.479516692	0.000000000	0.604999064
C	0.000000000	0.000000000	-2.037741296
C	0.000000000	0.000000000	-0.633956279

2f

Si	-2.307051000	-0.078505000	-0.001472000
Si	0.131523000	1.272892000	-0.008086000
C	-0.644196000	-0.500941000	-0.720236000
Si	2.048330000	-0.450493000	0.004114000
H	0.778481000	-0.177676000	-2.338366000
C	0.647439000	-0.340481000	-1.271126000
C	-0.645267000	-0.491634000	0.725432000
C	0.645666000	-0.324012000	1.275910000
H	0.775364000	-0.147462000	2.341129000

3f

C	0.000000000	1.242796503	0.603960473
C	0.000000000	0.682487001	1.900767480
H	0.000000000	-1.294960503	2.798741984
H	0.000000000	1.294960503	2.798741984
Si	0.000000000	0.000000000	-0.862044533
C	0.000000000	-0.682487001	1.900767480
Si	0.000000000	-2.335034505	-0.744138038
Si	0.000000000	2.335034505	-0.744138038
C	0.000000000	-1.242796503	0.603960473

4f

C	0.432533000	2.254506000	0.000000000
H	-1.719312000	2.519422000	0.000000000
C	-0.875491000	1.833054000	0.000000000
C	0.095724000	-0.413083000	0.000000000
Si	1.594225000	0.852001000	0.000000000
C	-1.061473000	0.436889000	0.000000000
Si	1.632909000	-1.382139000	0.000000000
H	0.703732000	3.304452000	0.000000000
Si	-1.674241000	-1.205200000	0.000000000

1g

Si	-2.325359000	-0.163185000	-0.000751000
Ge	0.167896000	1.418965000	-0.009075000
C	-0.647295000	-0.469721000	-0.722819000
Si	2.038578000	-0.466231000	0.004208000
H	0.778799000	-0.222841000	-2.351848000
C	0.646141000	-0.349479000	-1.279548000
C	-0.648306000	-0.460417000	0.727502000
C	0.644363000	-0.332948000	1.284433000
H	0.775473000	-0.192455000	2.355197000

2g

H	-2.906839000	-0.011738000	-0.062969000
Si	-0.606514000	1.141486000	-0.928104000
C	-1.824586000	-0.005319000	-0.028357000
H	4.310554000	-0.003939000	-0.023605000
Si	-0.605898000	-1.385343000	-0.496209000
C	3.246580000	-0.002767000	-0.017310000
Ge	-0.633498000	0.268676000	1.573512000
C	2.040618000	-0.001079000	-0.010081000
C	0.638876000	-0.000024000	-0.000976000

3g

4g

C	1.271339503	0.000000000	-0.868608344
C	0.682394001	0.000000000	-2.145494351
H	-1.286519503	0.000000000	-3.049836856
H	1.286519503	0.000000000	-3.049836856
Ge	0.000000000	0.000000000	0.731066165
C	-0.682394001	0.000000000	-2.145494351
Si	-2.402657006	0.000000000	0.436861164
Si	2.402657006	0.000000000	0.436861164
C	-1.271339503	0.000000000	-0.868608344

1h

Si	-2.337992000	-0.261038000	-0.000135000
Sn	0.200747000	1.649145000	-0.010680000
C	-0.648442000	-0.450601000	-0.723525000
Si	2.026610000	-0.487877000	0.004355000
H	0.778073000	-0.288367000	-2.366121000
C	0.643900000	-0.358475000	-1.288570000
C	-0.649469000	-0.441278000	0.727997000
C	0.642096000	-0.341911000	1.293617000
H	0.774766000	-0.257910000	2.370361000

3h

H	-2.924041000	0.182748000	0.069401000
Si	-0.594549000	1.101332000	-0.953379000
C	-1.847054000	0.070825000	0.027005000
H	4.326949000	0.075983000	0.029195000
Sn	-0.684682000	-1.710345000	-0.631735000
C	3.263450000	0.050900000	0.019165000
Si	-0.594082000	0.214749000	1.441572000
C	2.056425000	0.025235000	0.008700000
C	0.656879000	-0.011473000	-0.004023000

1i

Si	-2.339233000	-0.297749000	0.000099000
Pb	0.219780000	1.754880000	-0.011549000
C	-0.648861000	-0.447768000	-0.724328000
Si	2.020711000	-0.484075000	0.004362000
H	0.774654000	-0.317099000	-2.371657000
C	0.641788000	-0.368949000	-1.292609000
C	-0.649900000	-0.438432000	0.728822000
C	0.639968000	-0.352382000	1.297843000
H	0.771383000	-0.286738000	2.376316000

3i

H	-2.930013000	-0.185809000	0.154607000
Pb	-0.702964000	1.480982000	-1.228694000
C	-1.855529000	-0.075121000	0.063172000
H	4.333883000	-0.071686000	0.060788000
Si	-0.592376000	-1.348522000	-0.538164000
C	3.270532000	-0.050939000	0.042707000
Si	-0.591903000	0.281516000	1.425013000
C	2.062438000	-0.031555000	0.027103000
C	0.665225000	0.001089000	-0.000634000

1j

Ge	0.000000000	2.429114000	0.533069000
Ge	0.000000000	-2.429114000	0.533069000
C	0.000000000	1.243224000	-0.863348000
C	0.000000000	-1.243224000	-0.863348000
C	0.000000000	0.685080000	-2.159131000
H	0.000000000	-1.295676000	-3.058723000
C	0.000000000	-0.685080000	-2.159131000
Si	0.000000000	0.000000000	0.590769000
H	0.000000000	1.295676000	-3.058723000

3j

H	2.806677000	1.774498000	-0.000136000
Si	-2.953064000	-0.118305000	-0.000067000
H	0.911965000	3.282836000	-0.000157000
Ge	-0.689801000	-0.695622000	-0.000011000
C	1.815361000	1.316827000	-0.000081000
C	-1.653159000	1.168969000	0.000204000
C	0.751979000	2.205241000	-0.000093000
C	-0.529232000	1.741023000	0.000120000
Ge	1.793381000	-0.616673000	0.000021000

1k

C	0.427530000	2.265589000	0.000105000
H	-1.720690000	2.539587000	-0.000396000
C	-0.880893000	1.848385000	-0.000254000
C	0.067143000	-0.419401000	0.000376000
Si	1.552285000	0.834199000	0.000221000
C	-1.077211000	0.450323000	0.000011000
Ge	1.738475000	-1.435973000	-0.000567000
H	0.706069000	3.313139000	0.000220000
Si	-1.684103000	-1.195947000	0.000284000

2h

C	0.414012000	2.283000000	-0.000020000
H	-1.730864000	2.569459000	0.000070000
C	-0.896129000	1.872700000	0.000023000
C	0.037869000	-0.399213000	-0.000047000
Si	1.514668000	0.828742000	-0.000060000
C	-1.104059000	0.473085000	-0.000008000
Sn	1.892303000	-1.578197000	0.000093000
H	0.697256000	3.329127000	-0.000012000
Si	-1.696449000	-1.178802000	-0.000039000

4h

C	0.000000000	1.343466003	1.154841354
C	0.000000000	0.681234002	2.390120862
H	0.000000000	-1.260191003	3.312269366
H	0.000000000	1.260191003	3.312269366
Sn	0.000000000	0.000000000	-0.746398652
C	0.000000000	-0.681234002	2.390120862
Si	0.000000000	-2.561827006	-0.040401654
Si	0.000000000	2.561827006	-0.040401654
C	0.000000000	-1.343466003	1.154841354

2i

C	0.408960000	2.286836000	-0.000004000
H	-1.733447000	2.589237000	0.000009000
C	-0.903543000	1.886767000	0.000012000
C	0.011150000	-0.395805000	-0.000009000
Si	1.488928000	0.813906000	0.000007000
C	-1.122030000	0.486212000	0.000001000
Pb	1.986290000	-1.626904000	0.000006000
H	0.701086000	3.330479000	-0.000014000
Si	-1.708787000	-1.170826000	-0.000009000

4i

C	0.000000000	-1.392697503	-1.470708693
C	0.000000000	-0.681834502	-2.672711200
H	0.000000000	1.240949003	-3.607665703
H	0.000000000	-1.240949003	-3.607665703
Pb	0.000000000	0.000000000	0.594973313
C	0.000000000	0.681834502	-2.672711200
Si	0.000000000	2.623321506	-0.304298184
Si	0.000000000	-2.623321506	-0.304298184
C	0.000000000	1.392697503	-1.470708693

2j

H	2.099525000	2.836656000	0.000066000
Ge	-2.097455000	-0.197115000	-0.000089000
C	1.390875000	2.011253000	0.000045000
Ge	0.352321000	-0.748794000	0.000170000
C	1.827020000	0.675230000	-0.000106000
C	-0.698365000	0.975664000	-0.000040000
H	-0.454386000	3.148725000	0.000118000
C	0.033450000	2.176355000	0.000079000
Si	2.777233000	-0.767666000	-0.000190000

4j

Si	0.285470000	-0.621536000	-0.000249000
H	-3.284474000	1.562198000	0.000596000
C	1.199480000	1.144289000	-0.000336000
C	-2.273764000	1.150413000	0.000292000
Ge	2.583536000	-0.225521000	0.000136000
C	-1.250968000	2.083337000	0.000123000
C	0.048971000	1.662716000	-0.000404000
Ge	-2.133736000	-0.782592000	0.000007000
H	-1.448026000	3.154381000	0.000268000

2k

C	1.359244005534	0.105510771999	0.000000000000
H	1.497128802816	2.323475921394	0.000000000000
C	2.714100041155	-0.262496569732	0.000000000000
N	3.811462631557	-0.622821144836	0.000000000000
Pb	-0.254867477926	-0.070504001057	1.740427709033
Pb	-0.254867477926	-0.070504001057	-1.740427709033
C	-0.567282616815	1.485727841648	0.000000000000
C	0.850384848658	1.444517397726	0.000000000000
H	-1.136540759514	2.408158679370	0.000000000000

C	-0.691796000000	0.000000000000	-2.838378437460
Pb	2.276679000000	0.000000000000	0.290744562540
N	0.000000000000	0.000000000000	-0.675126437460
H	1.339453000000	0.000000000000	-3.702398437460
Pb	-2.276679000000	0.000000000000	0.290744562540
H	-1.339453000000	0.000000000000	-3.702398437460
C	1.114196000000	0.000000000000	-1.495769437460
C	-1.114196000000	0.000000000000	-1.495769437460
C	0.691796000000	0.000000000000	-2.838378437460

3k

Pb	-2.528523647579	-0.257559572686	0.000000000000
Pb	2.555654310021	0.018689444802	0.000000000000
H	-1.908847994114	2.450278211186	0.897553142562
C	-0.479513338443	-1.104867369149	0.000000000000
C	-0.118636082672	1.936119336300	0.000000000000
C	-1.511648188557	1.973008120948	0.000000000000
N	1.040251270333	1.844341915939	0.000000000000
C	0.746323874061	-1.228089687302	0.000000000000
H	-1.908847994114	2.450278211186	-0.897553142562

4k

Pb	-2.295550340166	-0.120790335707	0.000000000000
Pb	2.069319129768	-0.383806229422	0.000000000000
C	-0.564946263686	1.298070340464	0.000000000000
C	2.662650732912	2.010698213097	0.000000000000
H	-0.378435580574	3.464079926756	0.000000000000
H	3.731942812480	2.069512966968	0.000000000000
C	0.111841414759	2.500997124387	0.000000000000
C	1.480104674358	2.381184906951	0.000000000000
N	-0.043187470574	0.076838701119	0.000000000000

1m

Ge	-0.747591000	1.320929000	-0.403450000
Ge	2.385839000	-0.175737000	-0.098471000
H	-2.517472000	0.133221000	1.772364000
H	-0.342613000	1.257059000	2.576735000
C	-1.558492000	-0.054680000	1.297613000
C	0.451811000	-0.607790000	-0.184908000
C	-0.381733000	0.583722000	1.727363000
C	0.738665000	0.256585000	0.901168000
As	-1.355300000	-1.194073000	-0.235994000

2m

H	0.965234102	2.386945130	0.000000000
C	3.706755790	-0.216654913	0.000000000
Ge	-0.611613549	0.562245117	-1.500784500
H	4.761751248	-0.383191509	0.000000000
C	0.456891046	1.427456257	0.000000000
Ge	-0.611613549	0.562245117	1.500784500
As	-0.122341868	-1.354119206	0.000000000
C	2.517828941	-0.025446282	0.000000000
C	1.136650956	0.173719098	0.000000000

3m

C	-0.691065000	0.000000000	2.070749795
C	-1.300881000	0.000000000	0.794931795
As	0.000000000	0.000000000	-0.689397205
C	1.300881000	0.000000000	0.794931795
C	0.691065000	0.000000000	2.070749795
H	-1.279134000	0.000000000	2.981544795
H	1.279134000	0.000000000	2.981544795
Ge	-2.921638000	0.000000000	-0.156485205
Ge	2.921638000	0.000000000	-0.156485205

4m

H	-2.033135810	3.018047678	0.000000000
Ge	2.334199186	0.152028438	0.000000000
C	-1.277462580	2.240433559	0.000000000
Ge	-0.462181431	-1.687841392	0.000000000
H	0.499900657	3.466820780	0.000000000
C	0.079391832	2.466936295	0.000000000
C	0.176024683	0.080188530	0.000000000
As	-1.800100409	0.452626090	0.000000000
C	0.857756585	1.302702292	0.000000000

1n

Si	2.421002004	-0.257600959	0.000000000
H	-0.859855997	-0.277254767	-2.311607000
C	0.684921002	-0.296198857	0.719353000
C	-0.617941001	-0.349756781	-1.255965000
C	-0.617941001	-0.349756781	1.255965000
Si	-0.351042897	1.417395203	0.000000000
H	-0.859855997	-0.277254767	2.311607000
C	0.684921002	-0.296198857	-0.719353000
P	-1.865626012	-0.529018708	0.000000000

2n

C	0.686256000	0.000000000	1.901269562
C	1.230127000	0.000000000	0.607826562
C	-1.230127000	0.000000000	0.607826562
C	-0.686256000	0.000000000	1.901269562
H	1.307232000	0.000000000	2.790390562
H	-1.307232000	0.000000000	2.790390562
Si	2.333347000	0.000000000	-0.768052438
Si	-2.333347000	0.000000000	-0.768052438
P	0.000000000	0.000000000	-0.738278438

3n

Si	-2.269920153	0.184850320	0.000000000
H	2.453212277	2.087107221	0.000000000
Si	0.146784662	-2.012052684	0.000000000
C	1.530857746	1.518451459	0.000000000
C	-0.755472897	1.086897571	0.000000000
C	0.259762304	2.053462409	0.000000000
C	-0.284970786	-0.258773041	0.000000000
P	1.544957185	-0.223756530	0.000000000
H	0.070602422	3.121766253	0.000000000

4n

P	0.000000000	0.000000000	-2.993410413
H	0.000000000	-2.181303000	0.569383587
C	0.000000000	0.000000000	-1.453359413
C	0.000000000	-1.139001000	0.858031587
Si	-1.373619000	0.000000000	1.592269587
Si	1.373619000	0.000000000	1.592269587
C	0.000000000	0.000000000	-0.056381413
C	0.000000000	1.139001000	0.858031587
H	0.000000000	2.181303000	0.569383587

1p

Si	0.000000000	2.455749000	0.523706000
Si	0.000000000	-2.455749000	0.523706000
C	0.000000000	1.266258000	-0.766372000
C	0.000000000	-1.266258000	-0.766372000
H	0.000000000	1.296933000	-2.934104000
C	0.000000000	-0.686125000	-2.036596000
C	0.000000000	0.686125000	-2.036596000
H	0.000000000	-1.296933000	-2.934104000
As	0.000000000	0.000000000	0.752729000

2p

C	-0.334541000	-1.994993000	0.000000000
Si	1.870989000	2.441001000	0.000000000
C	1.880301000	0.597702000	0.000000000
H	-0.762825000	-2.996534000	0.000000000
C	1.052183000	-1.881297000	0.000000000
C	1.573262000	-0.632690000	0.000000000
Si	0.000000000	1.066092000	0.000000000
H	1.702271000	-2.752344000	0.000000000
As	-1.580622000	-0.602508000	0.000000000

3p

C	0.227901000	0.810002000	0.000000000
Si	-1.174924000	-0.153155000	1.412613000
C	1.298429000	1.705476000	0.000000000
H	-1.557041000	2.161006000	0.000000000
Si	-1.174924000	-0.153155000	-1.412613000

4p

H	1.116551000	4.311450000	0.000000000
H	-0.221005000	-2.781455000	0.000000000
Si	0.934154000	-0.678126000	1.317234000
C	0.934154000	3.258934000	0.000000000
C	0.051992000	-1.733250000	0.000000000

H	3.056165000	3.146405000	0.000000000
C	2.231710000	2.466772000	0.000000000
As	0.481819000	-1.144856000	0.000000000
C	-1.174924000	1.144610000	0.000000000

C	0.730116000	2.071454000	0.000000000
C	0.512961000	0.696805000	0.000000000
Si	0.934154000	-0.678126000	-1.317234000
As	-1.225067000	-0.251700000	0.000000000

5p

As	1.641915000	0.120656000	0.000000000
H	-4.826238000	0.788131000	0.000000000
H	-0.208936000	2.066134000	0.000000000
C	-0.105678000	0.984011000	0.000000000
C	-3.776340000	0.591060000	0.000000000
Si	-0.105678000	-0.679582000	1.403073000
C	-2.593200000	0.376939000	0.000000000
C	-1.222954000	0.080053000	0.000000000
Si	-0.105678000	-0.679582000	-1.403073000

6p

C	0.000000000	1.410649000	0.000000000
As	-1.729892000	0.832673000	0.000000000
C	-1.417450000	-1.051753000	0.000000000
H	-2.256630000	-1.739616000	0.000000000
Si	1.461262000	0.407060000	0.000000000
H	0.117345000	2.492865000	0.000000000
C	-0.154552000	-1.421193000	0.000000000
Si	2.959872000	-1.344030000	0.000000000
C	1.126979000	-1.456685000	0.000000000

1q

Si	0.000000000	2.600215000	0.179110000
Si	0.000000000	-2.600215000	0.179110000
C	0.000000000	1.323815000	-0.999674000
C	0.000000000	-1.323815000	-0.999674000
H	0.000000000	1.277085000	-3.149599000
C	0.000000000	-0.685322000	-2.237776000
C	0.000000000	0.685322000	-2.237776000
H	0.000000000	-1.277085000	-3.149599000
Sb	0.000000000	0.000000000	0.786932000

2q

C	0.583041000	-1.906702000	0.000000000
Si	1.492263000	3.077813000	0.000000000
C	1.947228000	1.294555000	0.000000000
H	0.531035000	-2.994170000	0.000000000
C	1.840311000	-1.326766000	0.000000000
C	1.945359000	0.027324000	0.000000000
Si	0.000000000	1.307217000	0.000000000
H	2.748277000	-1.927053000	0.000000000
Sb	-1.216993000	-0.882346000	0.000000000

3q

H	-4.551980000	0.812306000	0.000000000
H	2.716546000	0.701657000	0.000000000
Si	0.404661000	1.321890000	1.304388000
C	-3.485062000	0.767333000	0.000000000
C	1.632971000	0.690713000	0.000000000
C	-2.279847000	0.722006000	0.000000000
C	-0.890198000	0.682379000	0.000000000
Si	0.404661000	1.321890000	-1.304388000
Sb	0.404661000	-1.092186000	0.000000000

4q

C	0.085623000	1.098753000	0.000000000
Si	-1.321794000	0.129993000	1.428541000
C	1.127925000	2.025889000	0.000000000
H	-1.724982000	2.408388000	0.000000000
Si	-1.321794000	0.129993000	-1.428541000
H	2.841272000	3.519748000	0.000000000
C	2.039214000	2.814544000	0.000000000
Sb	0.476630000	-1.051059000	0.000000000
C	-1.321794000	1.400156000	0.000000000

5q

Sb	1.481244000	0.113653000	0.000000000
H	-5.217829000	0.690426000	0.000000000
H	-0.645853000	2.040912000	0.000000000
C	-0.505448000	0.963426000	0.000000000
C	-4.165685000	0.507835000	0.000000000
Si	-0.505448000	-0.693885000	1.417685000
C	-2.979773000	0.309005000	0.000000000
C	-1.603630000	0.036589000	0.000000000
Si	-0.505448000	-0.693885000	-1.417685000

6q

C	0.000000000	1.367792000	0.000000000
Sb	-1.660999000	0.224693000	0.000000000
C	-0.610488000	-1.607070000	0.000000000
H	-1.138487000	-2.555131000	0.000000000
Si	1.670313000	0.803239000	0.000000000
H	-0.170889000	2.443402000	0.000000000
C	0.693689000	-1.486872000	0.000000000
Si	3.619092000	-0.414216000	0.000000000
C	1.911577000	-1.072839000	0.000000000

1r

Si	0.000000000	2.643397000	-0.118915000
Si	0.000000000	-2.643397000	-0.118915000
C	0.000000000	1.355740000	-1.270942000
C	0.000000000	-1.355740000	-1.270942000
H	0.000000000	1.266127000	-3.406010000
C	0.000000000	-0.686257000	-2.485626000
C	0.000000000	0.686257000	-2.485626000
H	0.000000000	-1.266127000	-3.406010000
Bi	0.000000000	0.000000000	0.665307000

2r

C	1.948382000	0.242812000	0.000000000
Si	-1.617841000	-3.415975000	0.000000000
C	0.086683000	-2.726729000	0.000000000
H	2.820883000	0.893617000	0.000000000
C	2.165216000	-1.120971000	0.000000000
C	1.107900000	-1.977336000	0.000000000
Si	-1.085075000	-1.165208000	0.000000000
H	3.170857000	-1.539509000	0.000000000
Bi	0.000000000	1.184046000	0.000000000

3r

H	0.943409000	-4.716040000	0.000000000
H	-2.102300000	1.903499000	0.000000000
Si	-1.596117000	-0.432011000	1.298029000
C	0.535512000	-3.729352000	0.000000000
C	-1.596117000	0.945209000	0.000000000
C	0.066991000	-2.617204000	0.000000000
C	-0.480648000	-1.341408000	0.000000000
Si	-1.596117000	-0.432011000	-1.298029000
Bi	0.658985000	0.667053000	0.000000000

4r

C	0.053107000	-1.406615000	0.000000000
Si	1.457065000	-0.441041000	1.431813000
C	-0.996052000	-2.323335000	0.000000000
H	1.864749000	-2.711644000	0.000000000
Si	1.457065000	-0.441041000	-1.431813000
H	-2.721916000	-3.803269000	0.000000000
C	-1.915050000	-3.103893000	0.000000000
Bi	-0.379940000	0.844544000	0.000000000
C	1.457065000	-1.705014000	0.000000000

5r

Bi	0.336998000	1.131589000	0.000000000
H	-2.584608000	-5.045445000	0.000000000
H	-2.261523000	-0.277904000	0.000000000
C	-1.205159000	-0.530513000	0.000000000
C	-2.049241000	-4.121674000	0.000000000

6r

C	-1.389128000	-0.265001000	0.000000000
Bi	0.000000000	1.315817000	0.000000000
C	1.726499000	-0.063319000	0.000000000
H	2.743520000	0.314404000	0.000000000
Si	-1.031511000	-1.987838000	0.000000000

Si	0.336998000	-1.104730000	1.420145000
C	-1.451550000	-3.078093000	0.000000000
C	-0.720827000	-1.880742000	0.000000000
Si	0.336998000	-1.104730000	-1.420145000
H	-2.434952000	0.040195000	0.000000000
C	1.396758000	-1.325866000	0.000000000
Si	-0.075167000	-4.072265000	0.000000000
C	0.796691000	-2.466805000	0.000000000

1s

C	0.691497000	0.000000000	-2.381227315
C	1.121819000	0.000000000	-1.046762315
N	0.000000000	0.000000000	-0.208207315
C	-1.121819000	0.000000000	-1.046762315
C	-0.691497000	0.000000000	-2.381227315
H	1.339267000	0.000000000	-3.245408315
H	-1.339267000	0.000000000	-3.245408315
Ge	1.945757000	0.000000000	0.620444685
Ge	-1.945757000	0.000000000	0.620444685

2s

H	0.000000000	0.000000000	4.518160649
H	0.000000000	0.000000000	-4.051119304
N	0.000000000	0.000000000	3.520090615
C	0.000000000	0.000000000	-2.979795384
C	0.000000000	0.000000000	2.358916576
C	0.000000000	0.000000000	-1.757780474
Ge	0.000000000	1.449642000	-0.226441002
C	0.000000000	0.000000000	1.021586531
Ge	0.000000000	-1.449642000	-0.226441002

3s

Ge	-1.812222210	0.873793580	0.000000000
C	-1.145162548	-1.141609536	0.000000000
C	-0.053969701	-0.459039442	0.000000000
C	-2.515633690	-1.006399303	0.000000000
H	-3.627192548	-2.788210747	0.000000000
Ge	2.891214202	-0.071597973	0.000000000
N	1.201332560	-0.253340470	0.000000000
H	-4.605747100	-1.210770881	0.000000000
C	-3.642410702	-1.703118843	0.000000000

4s

H	-1.964267698	2.220455406	0.000000000
Ge	2.574598394	-0.156477524	0.000000000
H	0.205814447	2.729040455	0.000000000
N	-1.370641629	1.394426724	0.000000000
C	0.596267883	-0.719493824	0.000000000
C	-0.080304628	1.678773665	0.000000000
C	-0.634566802	-0.988117076	0.000000000
Ge	-2.421413789	-0.288216363	0.000000000
C	0.922079108	0.725348600	0.000000000

5s

H	0.000000000	2.189210000	0.433659000
H	0.000000000	-2.189210000	0.433659000
C	0.000000000	1.155857000	0.109394000
Ge	1.465349000	0.000000000	-0.737579000
Ge	-1.465349000	0.000000000	-0.737579000
N	0.000000000	0.000000000	3.545084000
C	0.000000000	-1.155857000	0.109394000
C	0.000000000	0.000000000	2.393417000
C	0.000000000	0.000000000	0.974825000

6s

H	1.151149000	2.406546000	0.000000000
Ge	-0.046990000	-1.473817000	0.000000000
H	3.383284000	1.334618000	0.000000000
C	2.382716000	-0.598290000	0.000000000
C	1.193793000	1.317190000	0.000000000
C	0.000000000	0.526614000	0.000000000
C	2.458702000	0.776065000	0.000000000
Ge	-1.659118000	1.349830000	0.000000000
N	1.978532000	-1.700434000	0.000000000

7s

Ge	0.041410000	2.944529000	0.000000000
Ge	-0.001825000	-2.846259000	0.000000000
C	1.151244000	0.223413000	0.000000000
C	0.659723000	-1.058325000	0.000000000
H	2.189898000	0.519236000	0.000000000
C	0.000000000	1.083971000	0.000000000
C	-1.154407000	0.237932000	0.000000000
H	-2.200899000	0.510328000	0.000000000
N	-0.742156000	-1.013738000	0.000000000

1t

C	0.687205000	0.000000000	2.214282606
C	1.237979000	0.000000000	0.923120606
P	0.000000000	0.000000000	-0.396414394
C	-1.237979000	0.000000000	0.923120606
C	-0.687205000	0.000000000	2.214282606
H	1.302029000	0.000000000	3.107451606
H	-1.302029000	0.000000000	3.107451606
Ge	2.469557000	0.000000000	-0.468621394
Ge	-2.469557000	0.000000000	-0.468621394

2t

H	-2.186340000	0.000000000	0.167257668
H	2.186340000	0.000000000	0.167257668
C	-1.151513000	0.000000000	-0.149145332
Ge	0.000000000	1.462175000	-0.982829332
Ge	0.000000000	-1.462175000	-0.982829332
P	0.000000000	0.000000000	3.680167668
C	1.151513000	0.000000000	-0.149145332
C	0.000000000	0.000000000	2.140345668
C	0.000000000	0.000000000	0.739566668

3t

H	0.482266086	-3.132036563	0.000000000
Ge	-0.435071076	0.791621494	0.000000000
H	-2.119063262	-3.027976414	0.000000000
C	-1.938519509	-0.868765841	0.000000000
C	-0.089564789	-2.207498470	0.000000000
C	0.540213963	-0.941435855	0.000000000
C	-1.455253466	-2.169231682	0.000000000
Ge	2.085239836	0.073819421	0.000000000
P	-2.744791698	0.531945765	0.000000000

4t

Ge	-2.817920000	1.228815000	0.000000000
Ge	2.856880000	-0.433095000	0.000000000
C	0.000000000	0.917682000	0.000000000
C	1.081730000	0.051132000	0.000000000
H	0.107545000	1.998397000	0.000000000
C	-1.237373000	0.226503000	0.000000000
C	-1.089375000	-1.189151000	0.000000000
H	-1.907593000	-1.899051000	0.000000000
P	0.534897000	-1.706624000	0.000000000

5t

H	-0.580266000	-3.329707000	0.000000000
Ge	-1.545431000	2.297367000	0.000000000
H	-2.545056000	-1.383830000	0.000000000

6t

Ge	-2.171467714	0.881760056	0.000000000
C	-1.598909424	-1.142251694	0.000000000
C	-0.568458968	-0.330732723	0.000000000

P	-0.183995000	-1.975654000	0.000000000
C	0.000000000	0.992082000	0.000000000
C	-1.548630000	-0.951155000	0.000000000
C	1.000146000	0.200656000	0.000000000
Ge	2.085513000	-1.346511000	0.000000000
C	-1.351082000	0.411906000	0.000000000
C	-2.946158284	-1.084854277	0.000000000
H	-4.111541465	-2.821071945	0.000000000
Ge	3.305195189	-0.082407231	0.000000000
P	1.161199719	-0.113112639	0.000000000
H	-5.046587275	-1.212399232	0.000000000
C	-4.098491603	-1.735588205	0.000000000

7t

H	0.000000000	0.000000000	4.958474000
H	0.000000000	0.000000000	-4.412190000
P	0.000000000	0.000000000	3.567158000
C	0.000000000	0.000000000	-3.341039000
C	0.000000000	0.000000000	2.014324000
C	0.000000000	0.000000000	-2.118280000
Ge	0.000000000	1.438240000	-0.586114000
C	0.000000000	0.000000000	0.687932000
Ge	0.000000000	-1.438240000	-0.586114000

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