Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information For

Planar Tetracoordinate Nitrogen in Main-Group Cationic Clusters

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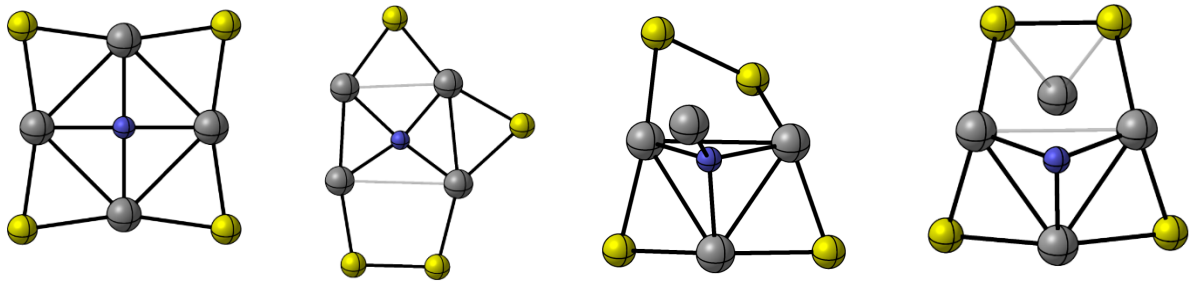
Computational Details

The potential energy surface (PES) of the N©$(XE)_4^+$ (X = Al, Ga, In; E = S, Se, Te, Po) systems was explored using the AUTOMATON program,[1] which applies a probabilistic cellular automata algorithm combined with genetic operations to generate and evolve structures toward global minima. Initial screening was performed at the PBE0[2]/SDDAll[4–8] level for both singlet and triplet states. The lowest energy structures were subsequently reoptimized using the PBE0-GD3/def2-TZVP[9] level of theory. All geometry optimizations and frequency calculations were performed using Gaussian 16.[10] Single-point energy refinements were carried out at the DLPNO-CCSD(T)[11–13]/CBS[14,15]//PBE0-GD3/def2-TZVP level.

Bonding analysis was conducted using the Adaptive Natural Density Partitioning (AdNDP) method,[16–18] as implemented in Multiwfn 3.8(dev).[19] This technique allows identification of classical and delocalized bonding elements, including multicenter bonds. All structures and AdNDP orbitals were visualized using VMD 1.9.3.[20]

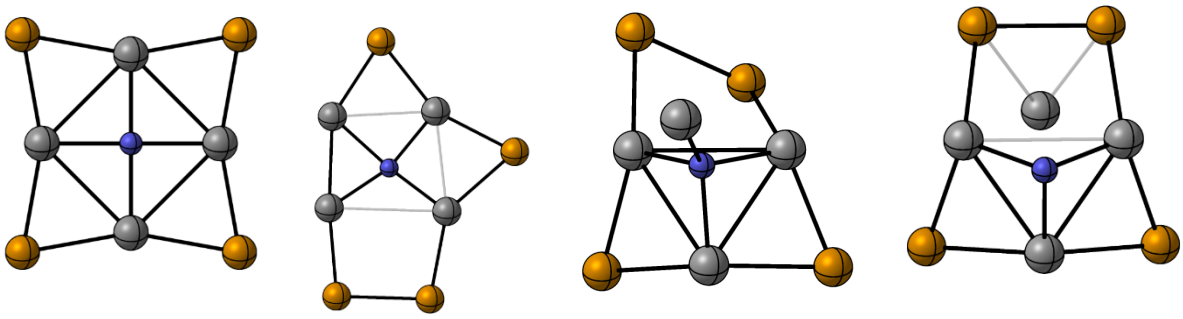
In addition, the Interacting Quantum Atoms (IQA) approach was applied to quantify interatomic interactions through energy decomposition.[21–23] IQA calculations were performed at the PBE0-GD3/def2-TZVP level using the AIMAll program.[24] The interaction energy (V_{IQA}^{int}) is expressed as the sum of Coulombic (V_C^{int}) and exchange-correlation (V_{XC}^{int}) terms, which respectively describe ionic and covalent contributions, respectively.

The magnetic response was evaluated through the calculation of magnetically induced current density using the GIMIC program.[25] The GIAO method was applied with the external magnetic field aligned perpendicular to the molecular plane (z-axis), ensuring origin-independent results.[26] The required perturbed density matrices were generated in Gaussian 16 using the BHandHLYP[27]/def2-TZVP level of theory. To complement the magnetic analysis the out-of-plane component of the induced magnetic field, B_Z^{ind}, was evaluated to characterize induced magnetic effects in real space.[28]



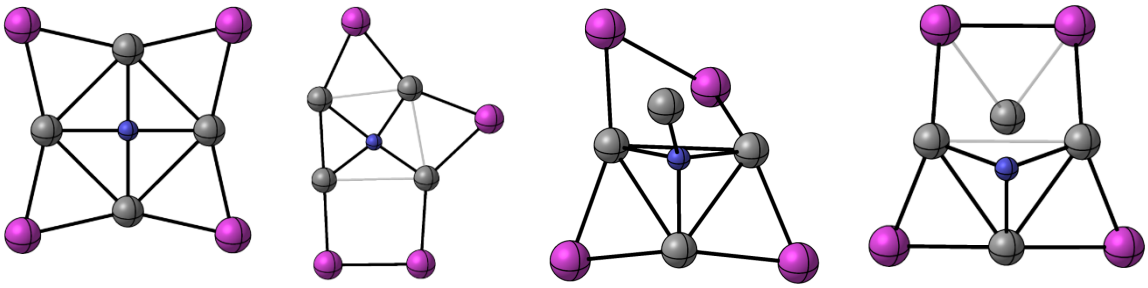
1a (D_{4h})	1b (C_s)	1c (C_1)	1d (C_s)
$^1A_{1g}$	$^1A'$	$^1A'$	$^1A'$
0.0	**72.0**	**82.7**	**95.5**
(0.0)	(69.0)	(80.4)	(90.7)

Figures S1. Global minimum and low-lying isomers of $N©Al_4S_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



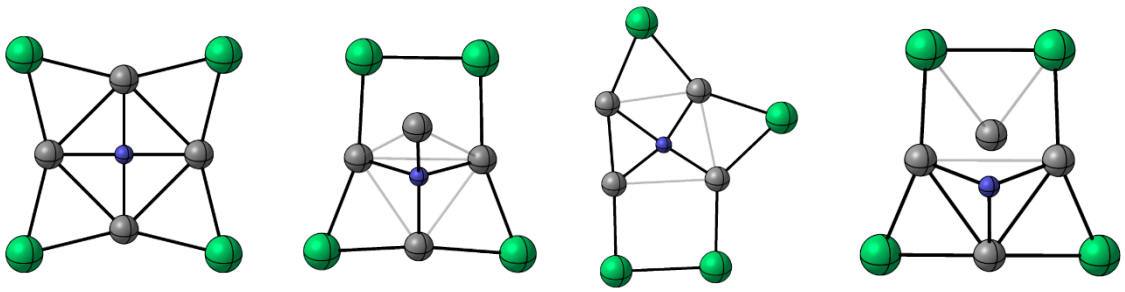
2a (D_{4h})	2b (C_s)	2c (C_1)	2d (C_s)
$^1A_{1g}$	$^1A'$	^1A	$^1A'$
0.0	**66.3**	**73.9**	**86.1**
(0.0)	(64.0)	(72.2)	(81.0)

Figure S2. Global minimum and low-lying isomers of $N©Al_4Se_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



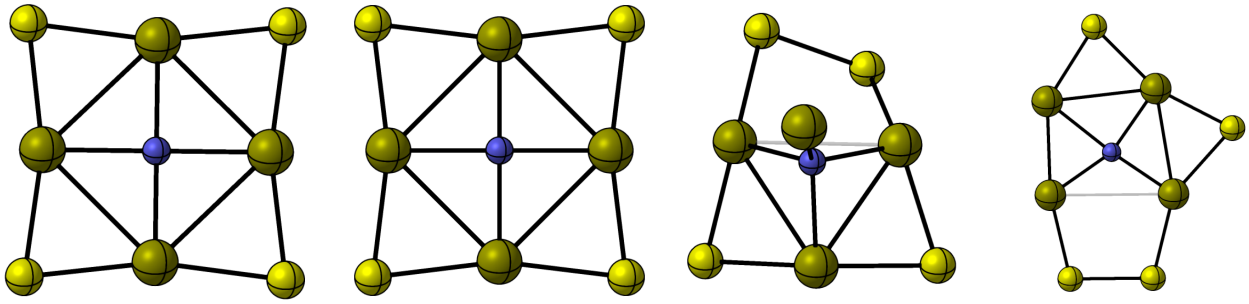
3a (D_{4h})	3b (C_s)	3c (C_1)	3d (C_s)
$^1A_{1g}$	$^1A'$	^1A	$^1A'$
0.0	**52.6**	**54.5**	**65.5**
(0.0)	(52.0)	(54.4)	(61.7)

Figure S3. Global minimum and low-lying isomers of N©$Al_4Te_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



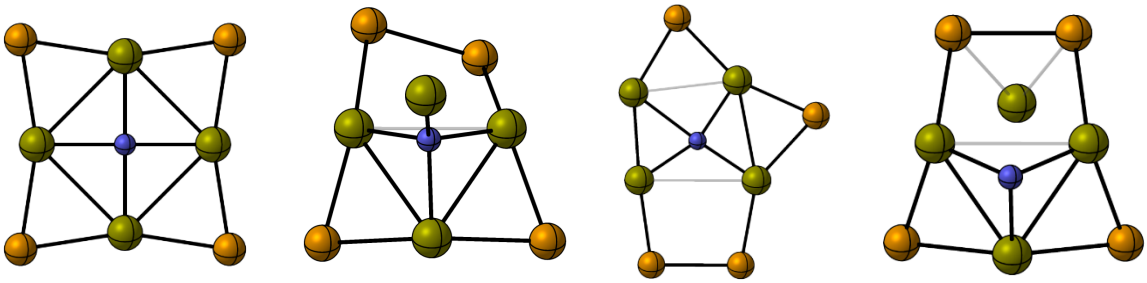
4a (D_{4h})	4b (C_s)	4c (C_s)	4d (C_s)
$^1A_{1g}$	$^1A'$	$^1A'$	$^1A'$
0.0	**45.8**	**47.8**	**57.7**
(0.0)	(46.0)	(46.8)	(53.6)

Figure S4. Global minimum and low-lying isomers of N©$Al_4Po_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



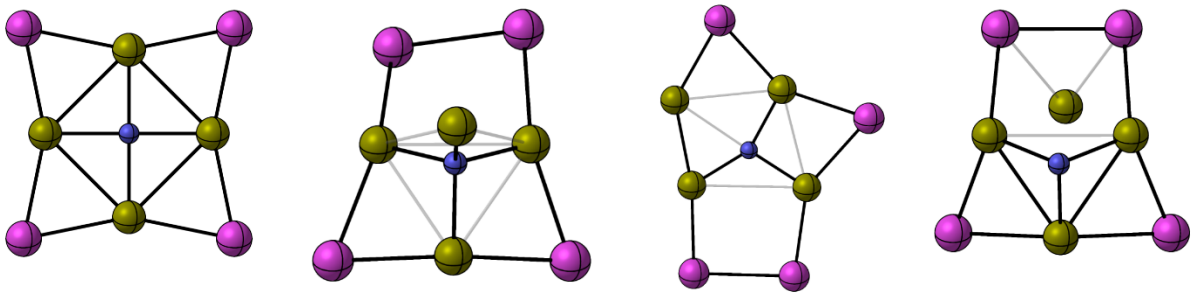
5a (C_{4v})	5b (D_{4h})	5c (C_1)	5d (C_s)
$^1A_1$	$^1A_{1g}$	^1A	$^1A'$
0.0	**0.03**	**48.5**	**49.1**
0.0	0.07	43.1	43.7

Figure S5. Global minimum and low-lying isomers of N©$Ga_4S_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



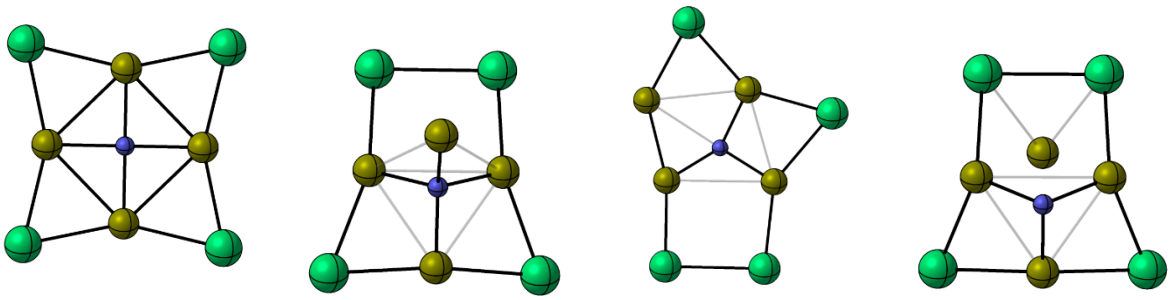
6a (D_{4h})	6b (C_1)	6c (C_1)	6d (C_s)
$^1A_{1g}$	^1A	^1A	$^1A'$
0.0	**43.4**	**46.4**	**55.5**
(0.0)	(38.7)	(41.6)	(47.7)

Figure S6. Global minimum and low-lying isomers of N©$Ga_4Se_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



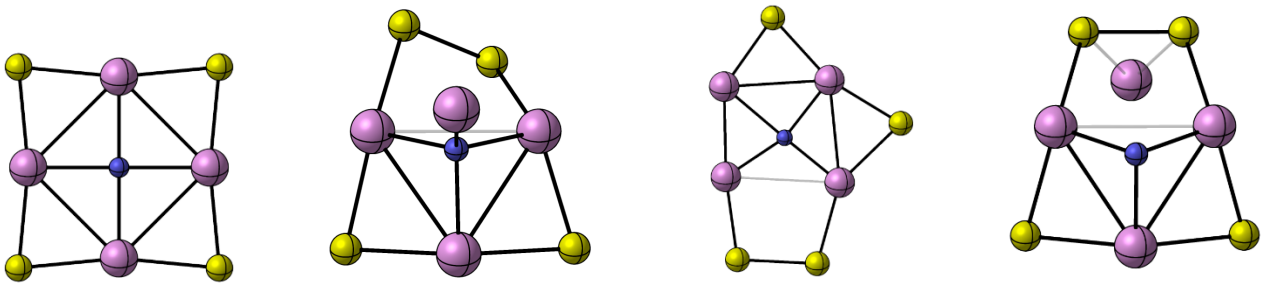
7a (D_{4h})	7b (C_1)	7c (C_s)	7d (C_s)
$^1A_{1g}$	^1A	$^1A'$	$^1A'$
0.0	**29.6**	**36.8**	**41.6**
(0.0)	(25.7)	(32.3)	(33.6)

Figure S7. Global minimum and low-lying isomers of N©$Ga_4Te_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



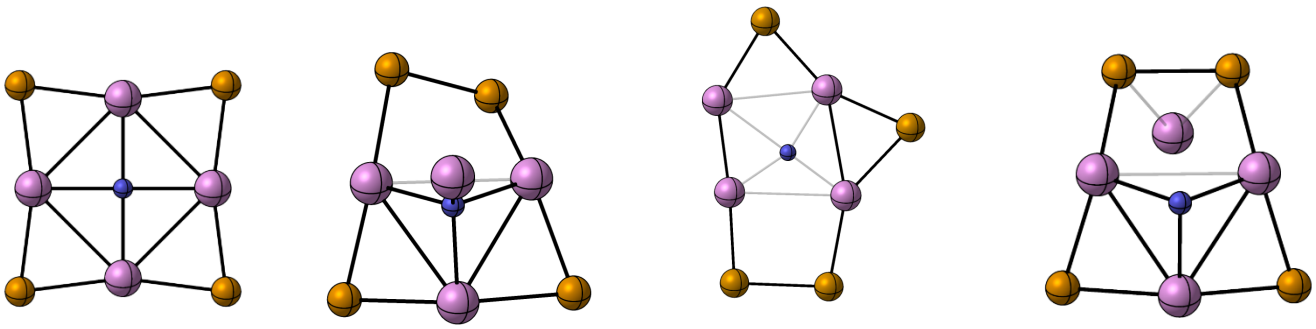
8a (D_{4h})	8b (C_s)	8c (C_s)	8d (C_s)
$^1A_{1g}$	$^1A'$	$^1A'$	$^1A'$
0.0	**23.0**	**32.0**	**34.7**
(0.0)	(19.5)	(28.0)	(27.4)

Figure S8. Global minimum and low-lying isomers of N©$Ga_4Po_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



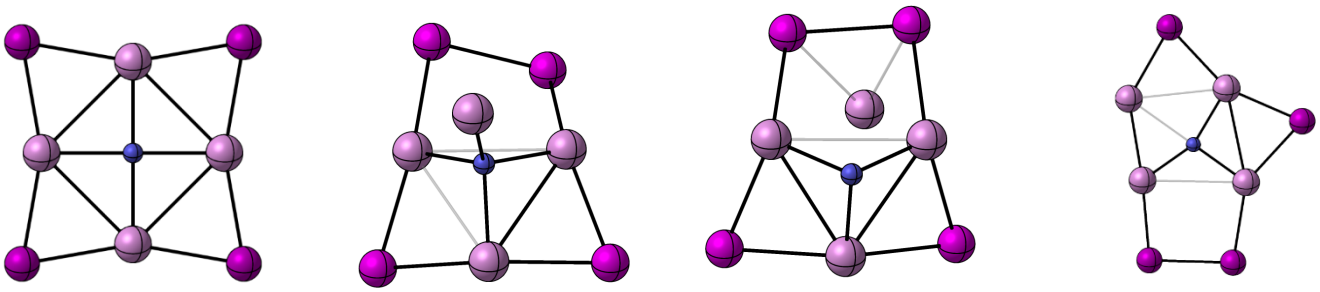
9a (D_{4h})	9b (C_1)	9c (C_1)	9d (C_s)
$^1A_{1g}$	^1A	^1A	$^1A'$
0.0	**29.2**	**38.6**	**43.2**
(0.3)	(27.2)	(33.7)	(39.0)

Figure S9. Global minimum and low-lying isomers of N©$In_4S_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



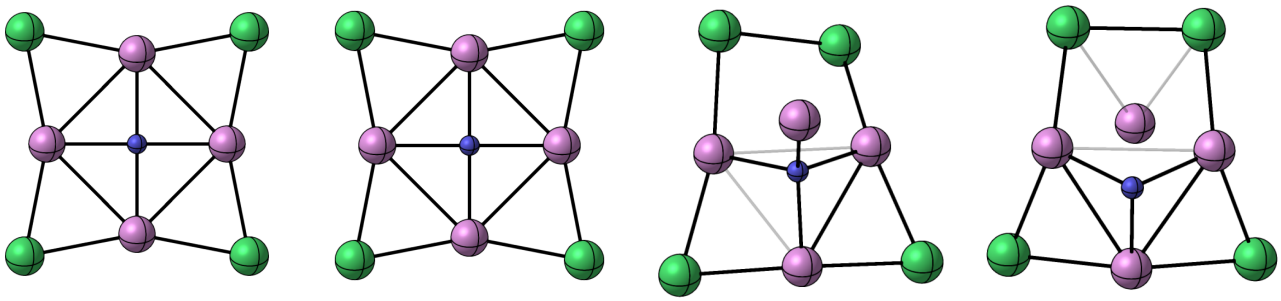
10a (D_{4h})	10b (C_1)	10c (C_s)	10d (C_s)
$^1A_{1g}$	^1A	$^1A'$	$^1A'$
0.0	**25.0**	**37.2**	**38.5**
(0.0)	(24.4)	33.8	(35.0)

Figure S10. Global minimum and low-lying isomers of N©$In_4Se_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



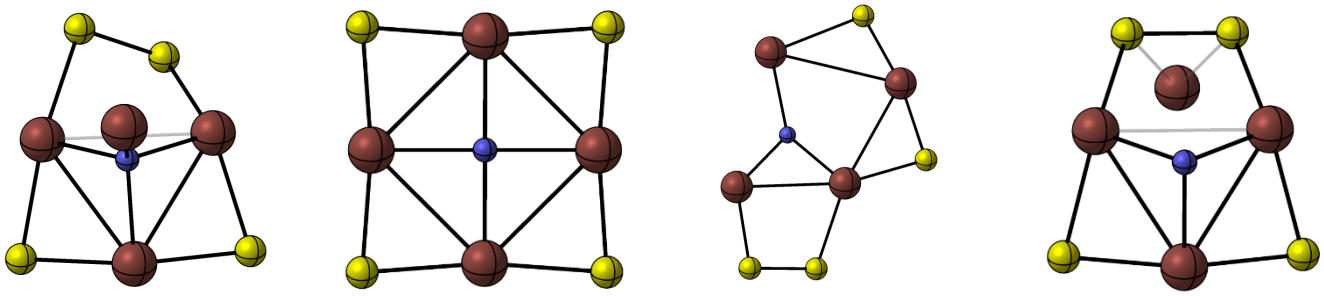
11a (D_{4h})	11b (C_1)	11c (C_s)	11d (C_s)
$^1A_{1g}$	^1A	$^1A'$	$^1A'$
0.0	**14.3**	**27.4**	**30.7**
(0.0)	(14.1)	(23.9)	(27.6)

Figure S11. Global minimum and low-lying isomers of N©$In_4Te_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



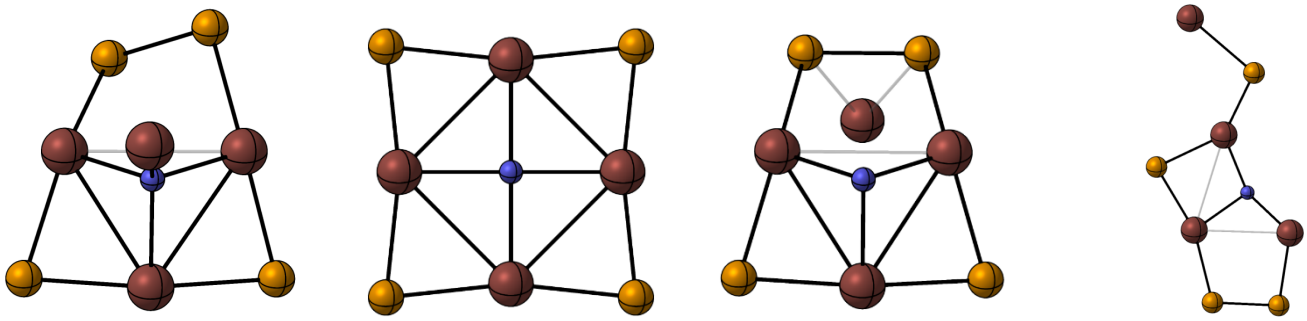
12a (D_{2d})	12b (D_{4h})	12c (C_1)	12d (C_s)
$^1A_1$	$^1A_{1g}$	^1A	$^1A'$
0.0	**0.3**	**10.2**	**23.3**
0.001	0.0	9.8	13.1

Figure S12. Global minimum and low-lying isomers of N©$In_4Po_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



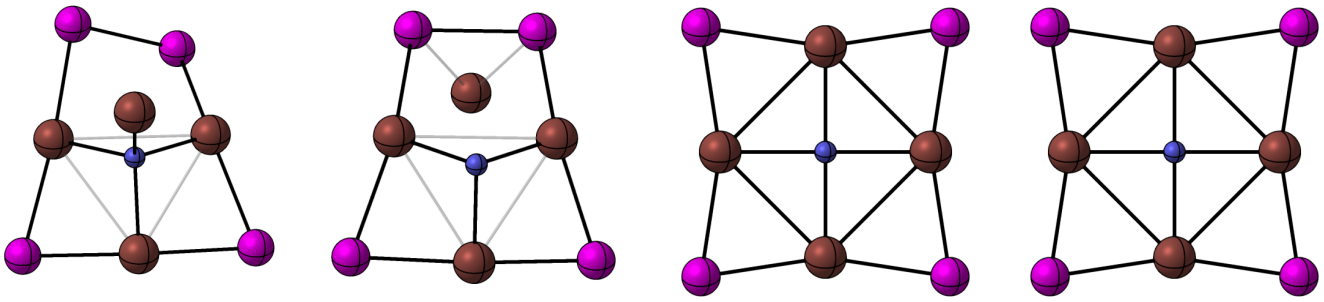
13a (C_1)	13b (D_{4h})	13c (C_1)	13d (C_s)
^{1}A	$^1A_{1g}$	^{1}A	^{1}A’
0.0	**5.9**	**10.0**	**12.9**
(0.0)	(6.5)	(7.6)	(12.7)

Figure S13. Global minimum and low-lying isomers of N©$Tl_4S_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



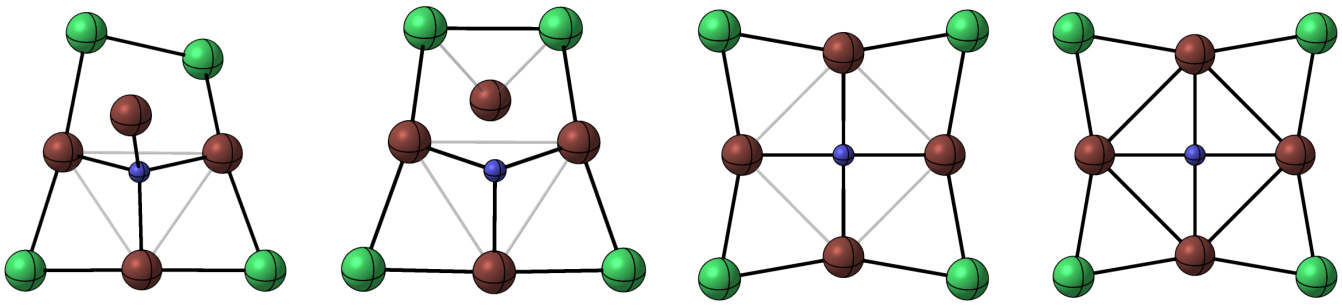
14a (C_1)	14b (D_{4h})	14c (C_s)	14d (C_1)
^{1}A	$^1A_{1g}$	^{1}A’	^{1}A
0.0	**6.9**	**12.5**	**14.5**
(0.0)	(6.2)	(10.8)	(9.8)

Figure S14. Global minimum and low-lying isomers of N©$Tl_4Se_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



15a (C_1)	15b (C_s)	15d (D_{4h})	15c (D_{2d})
^{1}A	^{1}A’	$^1A_{1g}$	$^1A_1$
0.0	**12.9**	**13.2**	**13.5**
0.0	9.8	13.1	12.9

Figure S15. Global minimum and low-lying isomers of N©$Tl_4Te_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).



16a (C_1)	16b (C_s)	16c (D_{2d})	16d (D_{4h})
^{1}A	^{1}A’	$^1A_1$	$^1A_{1g}$
0.0	**12.9**	**15.3**	**15.6**
0.0	9.8	15.4	16.0
(11.4)	(9.5)	(11.2)	(-20.4i)

Figure S16. Global minimum and low-lying isomers of N©$Tl_4Po_4^+$ cluster, their point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at DLPNO-CCSD(T)/CSB//PBE0-GD3/def2-TZVP (**in bold**) and PBE0-GD3/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).

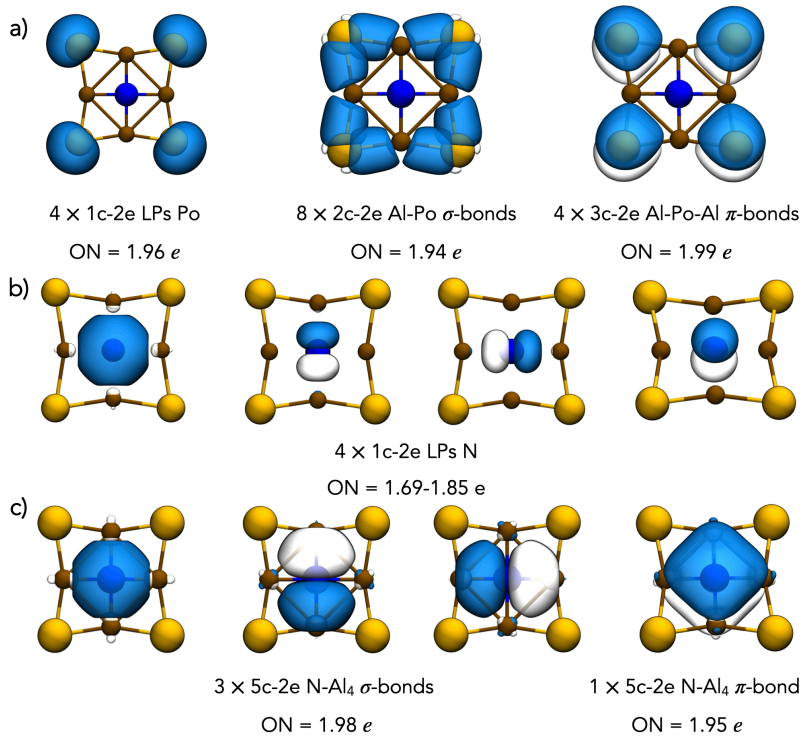


Figure S17. AdNDP bonding pattern of N©$(AlPo)_4^+$. a) AdNDP scheme with four 1c-2e E lone pairs, eight 2c-2e Al-E σ-bonds and four 3c-2e Al-E-Al π-bonds. b) Alternative pattern in line with an electrostatic model. c) Alternative pattern in line with delocalized bonding model. Occupation numbers are show.

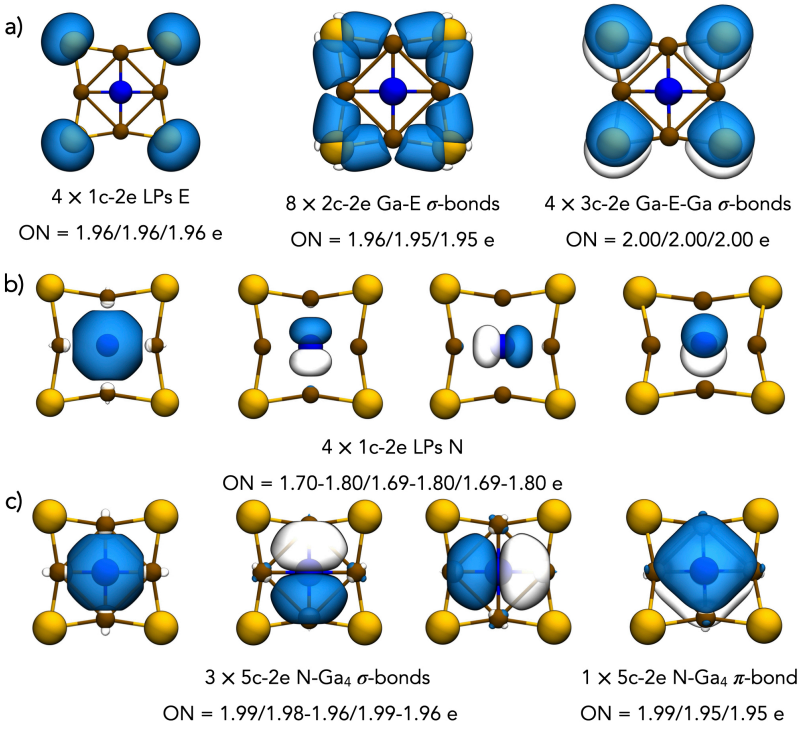


Figure S18. AdNDP bonding pattern of N©$(GaE)_4^+$ (E = Se–Po). a) AdNDP scheme with four 1c-2e E lone pairs, eight 2c-2e Ga-E σ-bonds and four 3c-2e Ga-E-Ga π-bonds. b) Alternative pattern in line with an electrostatic model. c) Alternative pattern in line with delocalized bonding model. Occupation numbers are show.

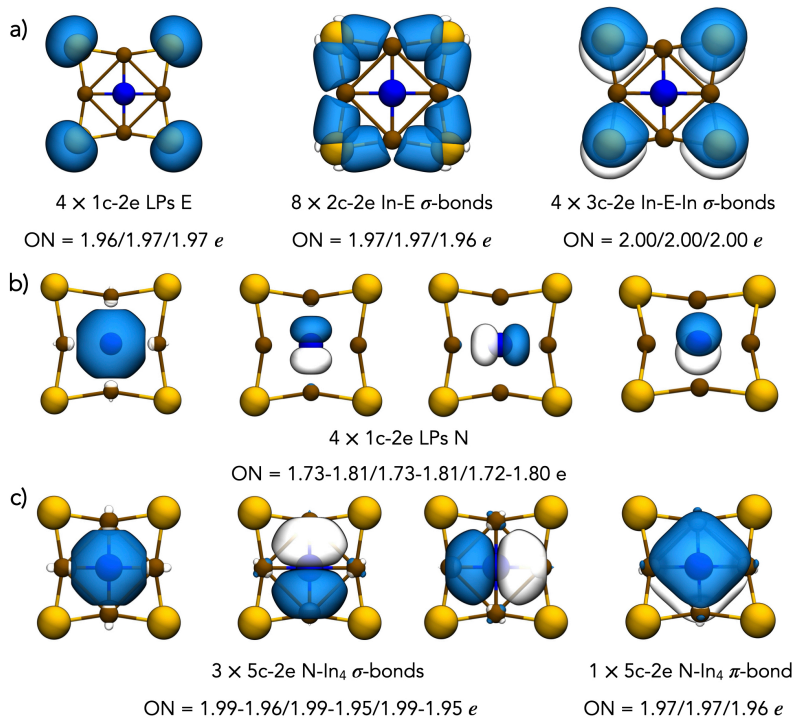


Figure S19. AdNDP bonding pattern of N©$(InE)_4^+$ (E = S–Te). a) AdNDP scheme with four 1c-2e E lone pairs, eight 2c-2e In-E σ-bonds and four 3c-2e In-E-In π-bonds. b) Alternative pattern in line with an electrostatic model. c) Alternative pattern in line with delocalized bonding model. Occupation numbers are show.

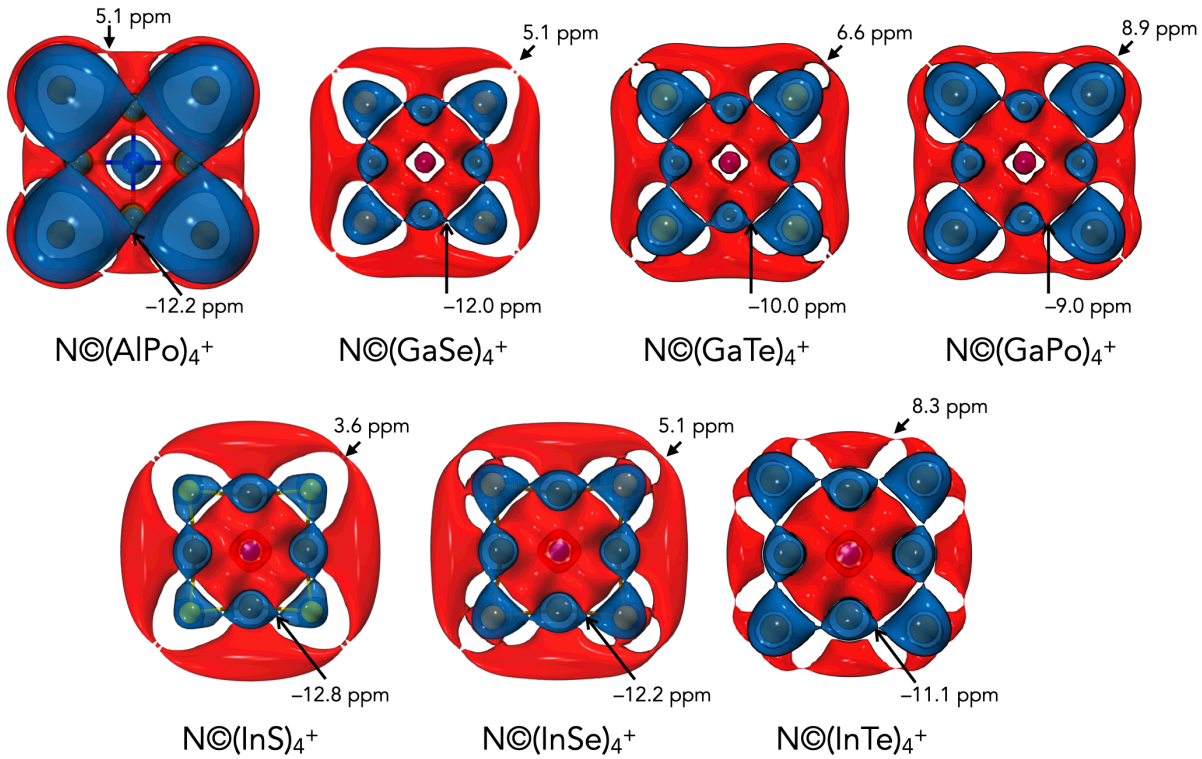


Figure S20. B_Z^{ind} isosurfaces for N©$(AlPo)_4^+$ and N©$(InE)_4^+$ (E = S–Te). Blue surfaces correspond to regions of magnetic shielding, while red surfaces indicate deshielding.

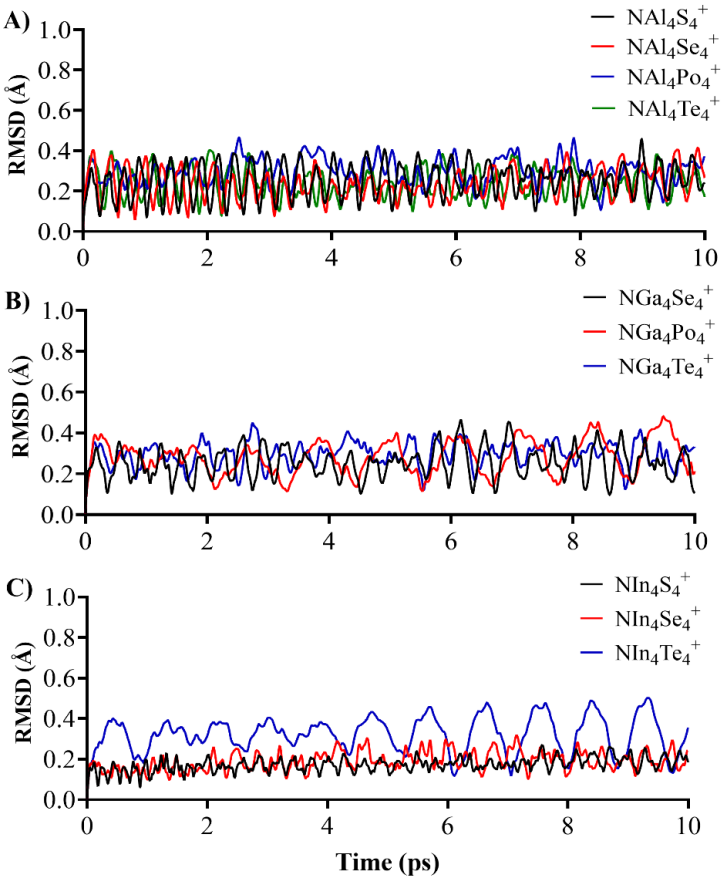
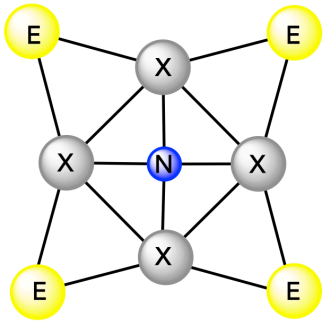


Figure S21. Born-Oppenheimer molecular dynamics (BO-MD) conducted at 500 K of minimum global of (a) N©$(AlE)_4^+$ (E= S-Po), (b) N©$(GaE)_4^+$ (E= Se-Po) and (c) N©$(InE)_4^+$ (E= S-Te).

Table S1. Lowest vibrational frequencies (ν, cm^{-1}) for D_{4h}-N©$(XE)_4^+$, where X represents group 13 elements and E denotes chalcogens at PBE0-GD3/def2-TZVP level.

System	ν_{min}	System	ν_{min}	System	ν_{min}
N©$(BO)_4^+$	494.6*i*	N©$(AlO)_4^+$	249.9*i*	N©$(GaO)_4^+$	219.6*i*
N©$(BS)_4^+$	193.5*i*	N©$(AlS)_4^+$	24.5	N©$(GaS)_4^+$	41.0*i*
N©$(BSe)_4^+$	113.4*i*	N©$(AlSe)_4^+$	41.5	N©$(GaSe)_4^+$	35.4
N©$(BTe)_4^+$	15.5	N©$(AlTe)_4^+$	24.7	N©$(GaTe)_4^+$	21.9
N©$(BPo)_4^+$	5.0	N©$(AlPo)_4^+$	17.4	N©$(GaPo)_4^+$	12.9
System	ν_{min}	System	ν_{min}		
N©$(InO)_4^+$	127.8*i*	N©$(TlO)_4^+$	104.6*i*		
N©$(InS)_4^+$	36.2	N©$(TlS)_4^+$	24.8		
N©$(InSe)_4^+$	27.4	N©$(TlSe)_4^+$	13.0		
N©$(InTe)_4^+$	10.5	N©$(TlTe)_4^+$	16.5*i*		
N©$(InPo)_4^+$	9.9*i*	N@$(TlPo)_4^+$	20.2*i*		

Table S2. Natural charges (q, |e|), Wiberg bond indices (WBI) and bond lengths (d, Å), lowest vibrational frequencies (ν, cm^{-1}), HOMO-LUMO energy gaps ($\Delta E_{H\text{-}L}$, eV), singlet-triplet energy differences ($\Delta E_{S\text{-}T}$, kcal·mol^{-1}) and T_1-diagnostic for global minimum of N©$(AlPo)_4^+$, N©$(GaE)_4^+$ (E = Se–Po) and N©$(InE)_4^+$ (E = S–Po) computed at the PBE0-GD3/def2-TZVP level.



System	q(N)	q(X)	q(E)	$WBI_{N\text{-}X}$	$WBI_{X\text{-}X}$	$WBI_{X\text{-}E}$	$d_{N\text{-}X}^*$	$d_{X\text{-}X}^*$	$d_{X\text{-}E}^*$	ν_{min}	$\Delta E_{H\text{-}L}$	$\Delta E_{S\text{-}T}$	T_1-diag
N©$(AlPo)_4^+$	–2.2	1.0	–0.2	0.29	0.11	1.08	1.90	2.68	2.60	17.4	4.5	70.7	0.011
N©$(GaSe)_4^+$	–2.1	1.3	–0.5	0.34	0.07	0.97	1.94	2.75	2.34	35.2	4.9	52.0	0.012
N©$(GaTe)_4^+$	–2.1	1.0	–0.2	0.34	0.09	1.04	1.97	2.78	2.52	21.9	4.1	40.5	0.012
N©$(GaPo)_4^+$	–2.1	0.8	–0.1	0.33	0.10	1.05	1.97	2.79	2.61	12.9	3.7	34.3	0.012
N©$(InS)_4^+$	–2.1	1.5	–0.7	0.35	0.05	0.85	2.15	3.04	2.39	36.1	4.2	42.6	0.019
N©$(InSe)_4^+$	–2.1	1.3	–0.5	0.36	0.06	0.92	2.17	3.09	2.51	27.9	4.2	45.3	0.013
N©$(InTe)_4^+$	–2.0	1.0	–0.3	0.36	0.07	0.99	2.19	3.09	2.69	10.9	3.8	41.3	0.014
N©$(InPo)_4^+$	–2.0	1.0	–0.2	0.36	0.08	1.00	2.19	3.10	2.77	9.9*i*	3.5	53.2	0.014

*The sum of Pyykkö's single bond radii for the N-Al, N-Ga, N-In, Al-S, Al-Se, Al-Te, Al-Po, Ga-Se, Ga-Te, Ga-Po, In-S, In-Se, In-Te, Al-Al, Ga-Ga and In-In bond are: 1.97, 1.95, 2.13, 2.29, 2.42, 2.62, 2.71, 2.40, 2.60, 2.69, 2.45, 2.58, 2.78, 2.52, 2.48 and 2.84 Å, respectively. The sums of van der Waals radii for the N-Al, N-Ga, N-In, Al-S, Al-Se, Al-Te, Ga-Se, Ga-Te, In-S, In-Se, In-Te, Al-Al, Ga-Ga and In-In bond are: 3.91, 3.98, 4.09, 4.14, 4.07, 4.24, 4.14, 4.31, 4.32, 4.25, 4.42, 4.50, 4.64 and 4.86 Å respectively.

Table S3. Energy components of IQA between atom pairs for N©$(AlPo)_4^+$, N©$(GaE)_4^+$ (E = Se–Po) and N©$(InE)_4^+$ (E = S–Po). 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^{-1}.

	N©$(AlPo)_4^+$	N©$(GaSe)_4^+$	N©$(GaTe)_4^+$	N©$(GaPo)_4^+$	N©$(InS)_4^+$	N©$(InSe)_4^+$	N©$(InTe)_4^+$	N©$(InPo)_4^+$
ΔE_{IQA}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
V_{IQA}^{int}(N-X)	**–959.8**	**–513.2**	**–442.6**	**–415.4**	**–429.4**	**–393.9**	**–345.0**	**–326.8**
V_C^{int}(N-X)	–909.4	–426.0	–355.0	–327.4	–345.2	–310.3	–261.9	–243.7
V_{XC}^{int}(N-X)	–50.4	–87.2	–87.6	–88.0	–84.2	–83.6	–83.1	–83.1
V_{IQA}^{int}(X-X)	**519.5**	**227.7**	**151.4**	**123.8**	**205.5**	**164.3**	**111.8**	**93.4**
V_C^{int}(X-X)	521.1	233.7	159.3	132.8	212.2	172.0	121.0	103.5
V_{XC}^{int}(X-X)	–1.6	–6.0	–7.9	–9.0	–6.7	–7.6	–9.2	–10.1
V_{IQA}^{int}(X-E)	**–463.9**	**–242.0**	**–166.6**	**–140.2**	**–244.5**	**–199.0**	**–146.6**	**–128.3**
V_C^{int}(X-E)	–392.3	–126.7	–52.7	–30.4	–130.1	–87.1	–37.9	–24.0
V_{XC}^{int}(X-E)	–71.6	–115.2	–113.9	–109.8	–114.4	–111.9	–108.8	–104.3

Cartesian Coordinates

Cartesian Coordinates for D_{4h}-N©$(XE)_4^+$, where X represents group 13 elements and E denotes chalcogens calculated at the PBE0-GD3/def2-TZVP level of theory.

1a (24.5)				1b (53.2)			
16	2.163793000	2.163793000	0.000000000	16	3.097910000	-0.891562000	0.000000000
13	0.000000000	1.850907000	0.000000000	16	1.687323000	-2.458248000	0.000000000
16	2.163793000	-2.163793000	0.000000000	16	-2.166503000	2.715935000	0.000000000
13	1.850907000	0.000000000	0.000000000	13	-0.200694000	-1.390229000	0.000000000
16	-2.163793000	2.163793000	0.000000000	13	-1.882608000	0.567728000	0.000000000
13	0.000000000	-1.850907000	0.000000000	13	1.800268000	0.842071000	0.000000000
13	-1.850907000	0.000000000	0.000000000	7	0.000000000	0.450170000	0.000000000
7	0.000000000	0.000000000	0.000000000	16	-2.386984000	-1.532769000	0.000000000
16	-2.163793000	-2.163793000	0.000000000	13	-0.002191000	2.404671000	0.000000000
1c (52.2)				1d (32.7)			
16	-2.365437000	-1.524704000	-0.294928000	16	-0.188527000	1.716113000	2.039701000
16	-0.661814000	1.920127000	-1.622944000	13	-2.329715000	-0.883159000	0.000000000
13	-0.325757000	-1.402316000	0.501172000	16	-0.188527000	-2.122532000	1.057207000
16	2.775054000	0.031348000	-0.057500000	13	0.843738000	-0.134929000	-1.445413000
16	1.547487000	-1.581647000	-0.670928000	7	1.714535000	0.419777000	0.000000000
13	0.851181000	0.993495000	-0.324553000	16	-0.188527000	-2.122532000	-1.057207000
13	-1.728751000	0.570065000	-0.288061000	13	0.843738000	-0.134929000	1.445413000
7	-0.349232000	0.391876000	1.035180000	13	0.647163000	1.927398000	0.000000000
13	-0.202828000	1.049131000	2.811022000	16	-0.188527000	1.716113000	-2.039701000
2a (41.7)				2b (29.2)			
34	2.276018000	2.276018000	0.000000000	34	-2.096382000	3.198674000	0.000000000
34	-2.276018000	-2.276018000	0.000000000	34	1.558589000	-2.523808000	0.000000000
13	0.000000000	1.868587000	0.000000000	13	0.146808000	2.638549000	0.000000000
13	0.000000000	-1.868587000	0.000000000	34	3.244073000	-0.831161000	0.000000000
13	1.868587000	0.000000000	0.000000000	13	-1.876712000	0.907507000	0.000000000
13	-1.868587000	0.000000000	0.000000000	13	-0.303692000	-1.177035000	0.000000000
34	-2.276018000	2.276018000	0.000000000	7	0.000000000	0.658182000	0.000000000
34	2.276018000	-2.276018000	0.000000000	13	1.827132000	0.964175000	0.000000000
7	0.000000000	0.000000000	0.000000000	34	-2.627338000	-1.253670000	0.000000000
2c (35.8)				2d (28.0)			
34	-2.720110000	-1.404659000	-0.205412000	34	-0.123067000	1.901607000	2.180282000
34	-0.859059000	2.465280000	-0.831392000	13	-2.262542000	-0.643563000	0.000000000
13	-0.480991000	-1.462429000	0.422195000	34	-0.123067000	-2.195200000	1.197845000
34	2.849029000	0.126873000	0.151427000	13	0.934758000	-0.064244000	-1.478237000
34	1.431807000	-1.479617000	-0.934257000	7	1.747532000	0.498068000	0.000000000
13	0.756967000	1.082165000	0.129799000	34	-0.123067000	-2.195200000	-1.197845000
13	-1.882621000	0.712430000	0.275344000	13	0.934758000	-0.064244000	1.478237000
7	-0.396655000	0.163183000	1.349019000	13	0.739520000	2.039576000	0.000000000
13	-0.014900000	0.343981000	3.205311000	34	-0.123067000	1.901607000	-2.180282000
3a (24.8)				3b (18.6)			
52	2.449477000	2.449477000	0.000000000	52	1.510378000	-2.724430000	0.000000000
52	-2.449477000	-2.449477000	0.000000000	52	-2.092699000	3.624051000	0.000000000
52	-2.449477000	2.449477000	0.000000000	52	3.516887000	-0.819770000	0.000000000
52	2.449477000	-2.449477000	0.000000000	52	-2.904457000	-1.145340000	0.000000000
13	0.000000000	1.891434000	0.000000000	13	-0.370617000	-1.068889000	0.000000000

13	0.000000000	-1.891434000	0.000000000	13	-1.866747000	1.118770000	0.000000000
13	1.891434000	0.000000000	0.000000000	13	1.846239000	1.017831000	0.000000000
13	-1.891434000	0.000000000	0.000000000	13	0.270689000	2.782112000	0.000000000
7	0.000000000	0.000000000	0.000000000	7	0.000000000	0.765388000	0.000000000
3c (30.0)				3d (28.4)			
52	-3.101839000	-1.429787000	0.025256000	52	-0.085512000	2.148923000	2.419208000
52	-0.934665000	2.749759000	-0.676613000	13	-2.171182000	-0.527475000	0.000000000
13	-0.615485000	-1.493582000	0.493387000	52	-0.085512000	-2.386597000	1.385186000
52	3.079464000	0.131325000	0.374429000	13	0.951374000	-0.008365000	-1.539513000
52	1.430628000	-1.614329000	-1.029991000	7	1.650038000	0.548401000	0.000000000
13	0.746429000	1.059025000	0.216945000	52	-0.085512000	-2.386597000	-1.385186000
13	-1.971744000	0.791146000	0.523882000	13	0.951374000	-0.008365000	1.539513000
7	-0.424553000	0.125917000	1.420655000	13	0.748147000	2.150309000	0.000000000
13	0.175057000	0.227737000	3.228492000	52	-0.085512000	2.148923000	-2.419208000
4a (17.4)				4b (7.6)			
84	2.521417000	2.521417000	0.000000000	13	-2.861174000	-0.292077000	0.000000000
84	2.521417000	-2.521417000	0.000000000	84	0.600885000	2.349269000	2.499802000
13	0.000000000	1.898402000	0.000000000	13	-0.274186000	0.069142000	-1.569136000
13	0.000000000	-1.898402000	0.000000000	84	-0.274186000	-2.543070000	1.482943000
84	-2.521417000	2.521417000	0.000000000	84	-0.274186000	-2.543070000	-1.482943000
84	-2.521417000	-2.521417000	0.000000000	13	-0.274186000	0.069142000	1.569136000
13	1.898402000	0.000000000	0.000000000	84	0.600885000	2.349269000	-2.499802000
13	-1.898402000	0.000000000	0.000000000	13	-0.213499000	2.304788000	0.000000000
7	0.000000000	0.000000000	0.000000000	7	-1.112268000	0.656507000	0.000000000
4c (12.5)				4d (26.2)			
84	3.637933000	-0.743060000	0.000000000	84	-0.058080000	2.267980000	2.514482000
84	1.497346000	-2.751890000	0.000000000	13	-2.081654000	-0.388857000	0.000000000
84	-2.111133000	3.833039000	0.000000000	84	-0.058080000	-2.438311000	1.470482000
13	-0.386851000	-0.974283000	0.000000000	13	0.975077000	0.030778000	-1.564152000
13	-1.864043000	1.238532000	0.000000000	7	1.620436000	0.588548000	0.000000000
13	1.851352000	1.096573000	0.000000000	84	-0.058080000	-2.438311000	-1.470482000
7	0.000000000	0.859608000	0.000000000	13	0.975077000	0.030778000	1.564152000
84	-3.008855000	-1.067188000	0.000000000	13	0.760092000	2.211587000	0.000000000
13	0.300737000	2.887411000	0.000000000	84	-0.058080000	2.267980000	-2.514482000
5a (52.9)				5b (-41.6i)			
16	2.190663000	2.190663000	-0.120564000	16	2.199943000	2.199943000	0.000000000
16	-2.190663000	-2.190663000	-0.120564000	16	-2.199943000	-2.199943000	0.000000000
31	0.000000000	1.919085000	0.044734000	31	0.000000000	1.928127000	0.000000000
31	-1.919085000	0.000000000	0.044734000	31	-1.928127000	0.000000000	0.000000000
31	1.919085000	0.000000000	0.044734000	31	1.928127000	0.000000000	0.000000000
7	0.000000000	0.000000000	0.309869000	7	0.000000000	0.000000000	0.000000000
31	0.000000000	-1.919085000	0.044734000	31	0.000000000	-1.928127000	0.000000000
16	-2.190663000	2.190663000	-0.120564000	16	-2.199943000	2.199943000	0.000000000
16	2.190663000	-2.190663000	-0.120564000	16	2.199943000	-2.199943000	0.000000000
5c (41.7)				5d (47.6)			
16	1.629773000	-2.025243000	-1.136658000	16	3.222788000	-0.819966000	0.000000000
16	0.344189000	-0.725880000	2.627286000	16	2.010315000	-2.530039000	0.000000000
31	-0.110595000	-0.644629000	-1.435159000	16	-2.335526000	2.351051000	0.000000000
16	-2.861872000	0.562055000	0.121061000	31	-0.032171000	-1.728686000	0.000000000
16	-2.289169000	-0.980347000	-1.176081000	31	-1.953980000	0.177854000	0.000000000

31	-0.934476000	0.404790000	1.196942000	31	1.774046000	0.814988000	0.000000000
31	1.433453000	-0.811047000	0.700200000	7	0.000000000	0.167917000	0.000000000
7	0.460434000	0.701343000	-0.147174000	16	-2.251252000	-1.992783000	0.000000000
31	1.147432000	2.528346000	-0.653581000	31	-0.121483000	2.242050000	0.000000000
6a (35.2)				6b (29.2)			
34	2.307268000	-2.307268000	0.000000000	31	-0.707906000	1.359078000	-0.114161000
34	-2.307268000	2.307268000	0.000000000	31	0.064256000	-1.542576000	0.182937000
34	-2.307268000	-2.307268000	0.000000000	34	2.266628000	-1.881761000	-0.610466000
31	0.000000000	1.946228000	0.000000000	7	0.388749000	0.190617000	1.008418000
31	0.000000000	-1.946228000	0.000000000	34	-2.885802000	0.522282000	-0.099190000
34	2.307268000	2.307268000	0.000000000	34	-2.062465000	-1.618889000	-0.765418000
31	1.946228000	0.000000000	0.000000000	34	1.073275000	2.359813000	-1.281679000
31	-1.946228000	0.000000000	0.000000000	31	0.442956000	0.419285000	3.011646000
7	0.000000000	0.000000000	0.000000000	31	1.876924000	0.399585000	-0.284593000
6c (34.5)				6d (9.6)			
34	3.239344000	-1.091225000	0.000000000	34	-0.126966000	1.854307000	2.218713000
34	1.584839000	-2.808587000	0.000000000	31	-2.348762000	-0.860798000	0.000000000
34	-1.996453000	3.059992000	0.000000000	34	-0.126966000	-2.303705000	1.196362000
31	-0.339981000	-1.520342000	0.000000000	31	0.917644000	-0.154027000	-1.510581000
31	-1.913513000	0.725927000	0.000000000	7	1.782319000	0.475037000	0.000000000
31	1.846072000	0.730875000	0.000000000	34	-0.126966000	-2.303705000	-1.196362000
7	0.000000000	0.352668000	0.000000000	31	0.917644000	-0.154027000	1.510581000
34	-2.700099000	-1.449775000	0.000000000	31	0.668028000	2.047360000	0.000000000
31	0.267440000	2.495076000	0.000000000	34	-0.126966000	1.854307000	-2.218713000
7a (21.9)				7b (11.8)			
52	2.473944000	2.473944000	0.000000000	31	-0.469171000	1.510781000	0.051820000
31	0.000000000	1.968365000	0.000000000	31	0.031565000	-1.583254000	0.171928000
52	-2.473944000	-2.473944000	0.000000000	52	2.439331000	-2.171195000	-0.452837000
31	0.000000000	-1.968365000	0.000000000	7	0.428555000	0.102522000	1.066323000
7	0.000000000	0.000000000	0.000000000	52	-2.928496000	0.977633000	-0.133829000
31	1.968365000	0.000000000	0.000000000	52	-2.323004000	-1.681158000	-0.696337000
31	-1.968365000	0.000000000	0.000000000	52	1.636866000	2.634396000	-0.841508000
52	-2.473944000	2.473944000	0.000000000	31	0.212398000	0.158365000	3.072625000
52	2.473944000	-2.473944000	0.000000000	31	2.099913000	0.294084000	0.026540000
7c (23.50)				7d (14.8)			
52	3.375324000	-1.303896000	0.000000000	52	-0.094632000	2.085722000	2.441042000
52	1.298880000	-3.142304000	0.000000000	31	-2.271599000	-0.755339000	0.000000000
52	-1.683412000	3.641609000	0.000000000	52	-0.094632000	-2.482112000	1.383455000
31	-0.557451000	-1.442634000	0.000000000	31	0.927347000	-0.099877000	-1.570387000
31	-1.776580000	1.093034000	0.000000000	7	1.677619000	0.527898000	0.000000000
31	1.832155000	0.631743000	0.000000000	52	-0.094632000	-2.482112000	-1.383455000
7	0.000000000	0.375284000	0.000000000	31	0.927347000	-0.099877000	1.570387000
52	-3.089503000	-1.051081000	0.000000000	31	0.673041000	2.165712000	0.000000000
31	0.667455000	2.745855000	0.000000000	52	-0.094632000	2.085722000	-2.441042000
8a (12.9)				8b (6.7)			
84	2.545381000	2.545381000	0.000000000	84	-0.158920000	-2.656692000	1.484223000
31	0.000000000	1.974876000	0.000000000	84	0.797130000	2.207172000	2.529045000
84	-2.545381000	-2.545381000	0.000000000	84	-0.158920000	-2.656692000	-1.484223000
31	0.000000000	-1.974876000	0.000000000	31	0.075953000	2.288158000	0.000000000
7	0.000000000	0.000000000	0.000000000	31	-0.158920000	-0.058183000	-1.601743000
31	1.974876000	0.000000000	0.000000000	84	0.797130000	2.207172000	-2.529045000

31	-1.974876000	0.000000000	0.000000000	7	-1.010360000	0.657732000	0.000000000
84	-2.545381000	2.545381000	0.000000000	31	-0.158920000	-0.058183000	1.601743000
84	2.545381000	-2.545381000	0.000000000	31	-2.988649000	0.115797000	0.000000000
8c (17.4)				8d (18.7)			
84	3.473896000	-1.231033000	0.000000000	84	0.072747000	-2.209130000	2.534451000
84	1.254478000	-3.168208000	0.000000000	31	2.162258000	0.574097000	0.000000000
84	-1.619456000	3.911717000	0.000000000	84	0.072747000	2.521661000	1.467919000
31	-0.601329000	-1.344243000	0.000000000	31	-0.950053000	0.051852000	-1.597018000
31	-1.725370000	1.265929000	0.000000000	7	-1.639735000	-0.579930000	0.000000000
31	1.823656000	0.720684000	0.000000000	84	0.072747000	2.521661000	-1.467919000
7	0.000000000	0.458073000	0.000000000	31	-0.950053000	0.051852000	1.597018000
84	-3.211121000	-0.868947000	0.000000000	31	-0.680379000	-2.240566000	0.000000000
31	0.779980000	2.929791000	0.000000000	84	0.072747000	-2.209130000	-2.534451000
9a (36.1)				9b (31.5)			
16	2.377861000	2.377861000	0.000000000	16	-0.054020000	-2.661657000	-1.526352000
16	-2.377861000	-2.377861000	0.000000000	16	-0.645095000	-1.119171000	2.715514000
49	0.000000000	2.150924000	0.000000000	49	-0.537929000	-0.284571000	-1.712687000
49	-2.150924000	0.000000000	0.000000000	16	-2.062005000	2.429103000	0.002836000
49	2.150924000	0.000000000	0.000000000	16	-2.568786000	0.997239000	-1.406506000
7	0.000000000	0.000000000	0.000000000	49	-0.830555000	0.875829000	1.372964000
49	0.000000000	-2.150924000	0.000000000	49	0.392251000	-1.828953000	0.670909000
16	-2.377861000	2.377861000	0.000000000	7	0.692561000	0.224780000	-0.024258000
16	2.377861000	-2.377861000	0.000000000	49	2.617674000	1.321335000	-0.257677000
9c (14.0)				9d (13.9)			
16	3.463730000	1.208835000	0.000000000	16	-0.906498000	1.743298000	2.282373000
16	2.189124000	2.854574000	0.000000000	49	-1.696036000	-2.814358000	0.000000000
16	-2.452956000	-2.505407000	0.000000000	16	0.935059000	-2.162314000	1.053381000
49	-0.032382000	1.998137000	0.000000000	49	0.935059000	0.267901000	-1.647432000
49	-2.186740000	-0.138804000	0.000000000	7	1.485196000	1.347724000	0.000000000
49	2.025629000	-0.682094000	0.000000000	16	0.935059000	-2.162314000	-1.053381000
7	0.000000000	-0.108734000	0.000000000	49	0.935059000	0.267901000	1.647432000
16	-2.439115000	2.210819000	0.000000000	49	-0.404904000	2.359668000	0.000000000
49	-0.054926000	-2.392341000	0.000000000	16	-0.906498000	1.743298000	-2.282373000
10a (28.0)				10b (21.5)			
34	2.487403000	2.487403000	0.000000000	49	0.476340000	-0.747043000	3.026303000
34	-2.487403000	-2.487403000	0.000000000	34	1.110412000	-2.308271000	-1.799443000
49	0.000000000	2.167854000	0.000000000	49	-0.114801000	1.740049000	0.219180000
49	-2.167854000	0.000000000	0.000000000	34	-3.164339000	-0.469020000	-0.148061000
49	2.167854000	0.000000000	0.000000000	34	-2.426849000	1.689734000	-0.787735000
7	0.000000000	0.000000000	0.000000000	49	-0.866157000	-1.458291000	-0.460438000
49	0.000000000	-2.167854000	0.000000000	34	2.251166000	2.219221000	-0.606618000
34	-2.487403000	2.487403000	0.000000000	49	2.000347000	-0.283322000	-0.588214000
34	2.487403000	-2.487403000	0.000000000	7	0.359426000	-0.256396000	0.854053000
10c (14.0)				10d (7.7)			
34	3.382334000	-1.607695000	0.000000000	34	-0.059741000	2.081421000	2.416028000
34	1.627046000	-3.205565000	0.000000000	49	-2.729724000	-1.599999000	0.000000000
34	-2.005705000	3.277575000	0.000000000	34	-0.059741000	-2.488139000	1.195597000
49	-0.419016000	-1.773971000	0.000000000	49	0.977364000	-0.142172000	-1.678750000
49	-2.127820000	0.771903000	0.000000000	7	1.875088000	0.599932000	0.000000000
49	2.088779000	0.506124000	0.000000000	34	-0.059741000	-2.488139000	-1.195597000
7	0.000000000	0.295315000	0.000000000	49	0.977364000	-0.142172000	1.678750000

34	-2.949541000	-1.572677000	0.000000000	49	0.672938000	2.363063000	0.000000000
49	0.420495000	2.610579000	0.000000000	34	-0.059741000	2.081421000	-2.416028000
11a (10.9)				11b (12.2)			
52	2.652365000	2.652365000	0.000000000	49	-0.161950000	0.279362000	3.181769000
52	2.652365000	-2.652365000	0.000000000	52	-1.592777000	2.770945000	-1.177267000
49	0.000000000	2.186870000	0.000000000	49	0.056283000	-1.763247000	0.062188000
49	0.000000000	-2.186870000	0.000000000	52	3.247461000	0.808758000	-0.129207000
52	-2.652365000	2.652365000	0.000000000	52	2.529495000	-1.712262000	-1.002993000
52	-2.652365000	-2.652365000	0.000000000	49	0.667998000	1.621035000	-0.188530000
49	2.186870000	0.000000000	0.000000000	52	-2.552262000	-2.329450000	-0.532834000
49	-2.186870000	0.000000000	0.000000000	49	-2.238125000	0.333922000	-0.177122000
7	0.000000000	0.000000000	0.000000000	7	-0.392243000	0.134547000	0.966105000
11c (10.7)				11d (17.1)			
52	-1.208999000	2.965540000	0.365752000	52	3.500878000	-1.797631000	0.000000000
49	1.567910000	0.360411000	2.291844000	52	1.325986000	-3.505740000	0.000000000
52	2.982220000	0.488211000	-0.664693000	52	-1.715915000	3.851449000	0.000000000
49	-0.534918000	-1.805368000	-0.845971000	49	-0.630840000	-1.660969000	0.000000000
7	-0.928715000	0.021552000	-1.695448000	49	-1.994333000	1.155495000	0.000000000
52	2.098223000	-2.048274000	0.000706000	49	2.064360000	0.428154000	0.000000000
49	0.447193000	1.459733000	-1.240393000	7	0.000000000	0.354201000	0.000000000
49	-2.393461000	0.576881000	-0.254910000	52	-3.316409000	-1.175898000	0.000000000
52	-2.885840000	-1.965901000	0.573048000	49	0.778853000	2.815427000	0.000000000
12a (13.3)				12b (-9.9i)			
84	2.719516000	2.719516000	0.000000000	84	2.723179000	2.723179000	0.000000000
84	-2.719516000	-2.719516000	0.000000000	84	-2.723179000	-2.723179000	0.000000000
49	0.000000000	2.185635000	0.157296000	49	0.000000000	2.192483000	0.000000000
49	-2.185635000	0.000000000	-0.157296000	49	-2.192483000	0.000000000	0.000000000
49	2.185635000	0.000000000	-0.157296000	49	2.192483000	0.000000000	0.000000000
7	0.000000000	0.000000000	0.000000000	7	0.000000000	0.000000000	0.000000000
49	0.000000000	-2.185635000	0.157296000	49	0.000000000	-2.192483000	0.000000000
84	-2.719516000	2.719516000	0.000000000	84	-2.723179000	2.723179000	0.000000000
84	2.719516000	-2.719516000	0.000000000	84	2.723179000	-2.723179000	0.000000000
12c (9.5)				12d (11.7)			
84	-2.711057000	-2.451376000	-0.262750000	84	-0.107163000	2.244187000	2.681018000
84	-1.986095000	2.861007000	-0.822066000	49	-2.378245000	-0.580023000	0.000000000
49	-0.015766000	-1.761218000	0.118148000	84	-0.107163000	-2.723641000	1.469686000
84	3.158502000	1.040374000	-0.068769000	49	1.077729000	-0.153615000	-1.739886000
84	2.547462000	-1.704742000	-0.928486000	7	1.815145000	0.634672000	0.000000000
49	0.451187000	1.702021000	-0.085769000	84	-0.107163000	-2.723641000	-1.469686000
49	-2.409637000	0.285679000	0.193078000	49	1.077729000	-0.153615000	1.739886000
7	-0.437544000	0.114926000	1.078600000	49	0.698315000	2.440431000	0.000000000
49	0.307332000	0.193794000	3.189721000	84	-0.107163000	2.244187000	-2.681018000
13a (23.1)				13b (24.8)			
81	-2.926765000	0.036512000	0.036415000	16	2.420652000	2.420652000	0.000000000
16	1.350667000	-0.353629000	-2.778451000	16	2.420652000	-2.420652000	0.000000000
81	0.604073000	-0.183038000	1.853333000	81	0.000000000	2.243776000	0.000000000
16	0.848538000	3.140610000	0.586473000	81	0.000000000	-2.243776000	0.000000000
16	1.860973000	1.988651000	1.897361000	16	-2.420652000	2.420652000	0.000000000
81	0.619071000	1.438145000	-1.229517000	16	-2.420652000	-2.420652000	0.000000000
16	1.179291000	-2.580756000	1.348447000	81	2.243776000	0.000000000	0.000000000
81	0.718534000	-1.721466000	-0.865648000	81	-2.243776000	0.000000000	0.000000000

7	-0.577067000	-0.042913000	-0.031778000	7	0.000000000	0.000000000	0.000000000
13c (17.2)				13d (11.3)			
16	4.357500000	-0.547052000	-0.290064000	16	-0.900844000	-1.884860000	2.338793000
16	3.210167000	-2.106007000	0.320675000	81	3.399160000	0.658988000	0.000000000
16	-3.687882000	0.817971000	0.048965000	16	1.048763000	2.173571000	1.040675000
81	0.757480000	-1.445200000	-0.118153000	81	-0.900844000	0.598762000	-1.696718000
81	-2.629298000	-1.174484000	0.050681000	7	-2.111936000	0.201608000	0.000000000
81	2.546414000	1.081105000	0.100926000	16	1.048763000	2.173571000	-1.040675000
7	0.503593000	0.699675000	-0.094913000	81	-0.900844000	0.598762000	1.696718000
16	-1.153164000	-3.005987000	0.019281000	81	-1.473395000	-1.987993000	0.000000000
81	-1.256708000	2.434374000	-0.044779000	16	-0.900844000	-1.884860000	-2.338793000
14a (16.4)				14b (12.7)			
81	-0.337631000	-2.543843000	1.692254000	34	2.533346000	2.533346000	0.000000000
34	-2.194246000	2.182795000	1.091830000	34	2.533346000	-2.533346000	0.000000000
81	0.979382000	-0.630715000	-1.519245000	81	0.000000000	2.262548000	0.000000000
34	2.647324000	1.922797000	0.457130000	81	0.000000000	-2.262548000	0.000000000
34	3.293563000	-0.113939000	-0.464065000	34	-2.533346000	2.533346000	0.000000000
81	0.273681000	1.329370000	1.310337000	34	-2.533346000	-2.533346000	0.000000000
34	-1.138720000	-0.407657000	-2.994424000	81	2.262548000	0.000000000	0.000000000
81	-1.987766000	0.393489000	-0.712643000	81	-2.262548000	0.000000000	0.000000000
7	-0.258625000	-0.609762000	0.356705000	7	0.000000000	0.000000000	0.000000000
14c (10.9)				14d (6.8)			
34	-0.823624000	2.060017000	2.475870000	34	4.888681000	-0.876627000	0.132486000
81	-1.814113000	-2.955859000	0.000000000	34	4.250053000	1.213981000	-0.698025000
34	0.996131000	-2.355216000	1.187173000	34	-3.158308000	-1.673035000	-0.092071000
81	0.996131000	0.272675000	-1.724519000	81	1.801981000	1.483616000	0.103719000
7	1.488692000	1.399627000	0.000000000	81	-1.233503000	-0.181172000	0.171510000
34	0.996131000	-2.355216000	-1.187173000	81	2.464183000	-1.780531000	0.012475000
81	0.996131000	0.272675000	1.724519000	7	0.893413000	-0.540531000	0.411468000
81	-0.451621000	2.537374000	0.000000000	34	-0.555457000	2.364293000	0.275662000
34	-0.823624000	2.060017000	-2.475870000	81	-5.387017000	0.093036000	-0.162939000
15a (8.0)				15b (11.1)			
52	2.493160000	-2.464675000	0.476383000	52	-0.677800000	2.342126000	2.687400000
52	1.658702000	2.740545000	1.354927000	81	-2.041799000	-2.902195000	0.000000000
81	-0.201496000	-1.864985000	0.090815000	52	0.924222000	-2.601730000	1.379916000
52	-3.352075000	0.749433000	0.345343000	81	0.924222000	0.210743000	-1.779460000
52	-2.679427000	-1.727461000	1.267805000	7	1.425137000	1.237373000	0.000000000
81	-0.748589000	1.672085000	0.504596000	52	0.924222000	-2.601730000	-1.379916000
81	2.260448000	0.260211000	0.327333000	81	0.924222000	0.210743000	1.779460000
7	0.284874000	0.134004000	-0.764273000	81	-0.246200000	2.707093000	0.000000000
81	-0.128299000	0.371877000	-3.067953000	52	-0.677800000	2.342126000	-2.687400000
15c (-16.5i)				15d (16.6)			
52	2.701489000	2.701489000	0.000000000	52	2.692050000	2.692050000	0.000000000
52	-2.701489000	-2.701489000	0.000000000	52	-2.692050000	-2.692050000	0.000000000
81	0.000000000	2.286671000	0.000000000	81	2.268775000	0.000000000	0.259259000
81	-2.286671000	0.000000000	0.000000000	81	0.000000000	-2.268775000	-0.259259000
81	2.286671000	0.000000000	0.000000000	81	0.000000000	2.268775000	-0.259259000
7	0.000000000	0.000000000	0.000000000	7	0.000000000	0.000000000	0.000000000
81	0.000000000	-2.286671000	0.000000000	81	-2.268775000	0.000000000	0.259259000
52	-2.701489000	2.701489000	0.000000000	52	2.692050000	-2.692050000	0.000000000
52	2.701489000	-2.701489000	0.000000000	52	-2.692050000	2.692050000	0.000000000

16a (11.4)				16b (9.5)			
84	2.643601000	2.555481000	-0.307051000	84	0.071032000	2.528504000	2.778475000
84	1.973089000	-2.865571000	-1.017589000	81	-2.842922000	-2.028061000	0.000000000
81	-0.114792000	1.848139000	-0.048359000	84	0.071032000	-2.829279000	1.465811000
84	-3.287361000	-0.966871000	-0.181427000	81	0.910646000	-0.061401000	-1.803389000
84	-2.686508000	1.686541000	-1.195759000	7	1.647780000	0.761047000	0.000000000
81	-0.556109000	-1.762660000	-0.330272000	84	0.071032000	-2.829279000	-1.465811000
81	2.427652000	-0.247420000	-0.021395000	81	0.910646000	-0.061401000	1.803389000
7	0.370625000	-0.116196000	0.888956000	81	0.584577000	2.708923000	0.000000000
81	-0.381337000	-0.252767000	3.125096000	84	0.071032000	2.528504000	-2.778475000
16c (11.2)				16d (-20.4i)			
84	2.759357000	2.759357000	0.000000000	84	2.775072000	2.775072000	0.000000000
84	-2.759357000	-2.759357000	0.000000000	84	-2.775072000	-2.775072000	0.000000000
81	0.000000000	2.263858000	0.332711000	81	0.000000000	2.292812000	0.000000000
81	-2.263858000	0.000000000	-0.332711000	81	-2.292812000	0.000000000	0.000000000
81	2.263858000	0.000000000	-0.332711000	81	2.292812000	0.000000000	0.000000000
7	0.000000000	0.000000000	0.000000000	7	0.000000000	0.000000000	0.000000000
81	0.000000000	-2.263858000	0.332711000	81	0.000000000	-2.292812000	0.000000000
84	-2.759357000	2.759357000	0.000000000	84	-2.775072000	2.775072000	0.000000000
84	2.759357000	-2.759357000	0.000000000	84	2.775072000	-2.775072000	0.000000000

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