

Supporting Information

Structure and Bonding in $[\text{Sb}@\text{In}_8\text{Sb}_{12}]^{3-}$ and $[\text{Sb}@\text{In}_8\text{Sb}_{12}]^{5-}$

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Supporting Information
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1. Experimental Procedures

All manipulations and reactions were performed in a nitrogen atmosphere using standard Schlenk or glovebox techniques. En (Aldrich, 99%) and DMF (Aldrich, 99.8%) were freshly distilled by CaH_2 prior to use. Tol (Aldrich, 99.8%) was distilled from sodium/benzophenone under nitrogen and stored under nitrogen. 2,2,2-crypt (4,7,13,16,21,24-Hexaoxa-1,10-diazabicyclo (8.8.8) hexacosane, purchased from Sigma-Aldrich, 98%) was dried in vacuum for one day prior to use. K_5Sb_4 was synthesized by heating a stoichiometric mixture of the elements at 800°C for two days in a niobium tube. $\text{In}(\text{benzyl})_3$ was prepared according to literature methodology.¹

X-ray Diffraction. Suitable single crystals were selected for X-ray diffraction analyses. Crystallographic data were collected on a Bruker Apex II CCD diffractometer with graphite-monochromated Mo $\text{K}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). Data processing was accomplished with the SAINT program. Structures were solved using direct methods and then refined using SHELXL-2014 and Olex2 2-5 to convergence, in which all the non-hydrogen atoms were refined anisotropically during the final cycles. All hydrogen atoms of the organic molecule were placed by geometrical considerations and were added to the structure factor calculation. Positional disorder was found in the cluster site in compound **1**, and this was modeled accordingly (see Figure S2 and Computational Details). A summary of the crystallographic data for these complexes is listed in Table S1, and selected bond distances are given in Tables S2.

Electrospray Ionization Mass Spectrometry (ESI-MS) Investigations. ESI-MS of the single crystal of compound **1** were performed on Agilent Technologies ESI-TOF-MS (6224). The samples were made up inside a glovebox under an inert atmosphere and rapidly transferred to the spectrometer in an air-tight syringe by direct infusion with a Harvard syringe pump at 15 uL/min .

Energy Dispersive X-ray (EDX) Spectroscopy. EDX Analysis was performed using a scanning electron microscope (Hitachi S-4800) equipped with a Bruker AXS XFlash detector 4010. Data acquisition was performed with an acceleration voltage of 20 kV and an accumulation time of 150 s .

Synthesis of $[\text{K}(\text{2,2,2-crypt})]_4[\text{Sb}@\text{In}_8\text{Sb}_{12}]$ (**1**):

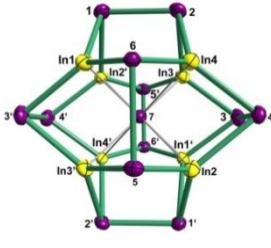
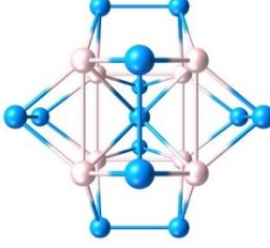
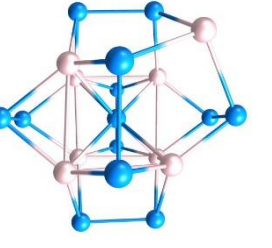
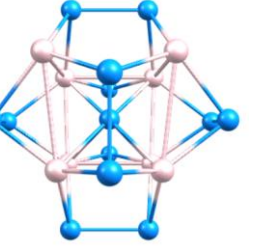
K_5Sb_4 (68.2 mg, 0.1 mmol) was weighed into a 10 mL vial inside a glovebox and dissolved in en (3 mL). After stirring for three hours, the resulting dark brown solution was filtered onto a mixture of $\text{In}(\text{benzyl})_3$ (35.2mg, 0.10mmol) and 2,2,2-crypt (151 mg, 0.4 mmol) and allowed to stir for a further two hours. The resulting black solution was filtered through glass wool and transferred to a test tube, then carefully layered by toluene (5 mL) to allow for crystallization. Small black plate-like crystals of $[\text{K}(\text{2,2,2-crypt})]_4[\text{Sb}@\text{In}_8\text{Sb}_{12}]$ (**1**), were isolated after two weeks in approximately 18% yield in total (based on precursor $\text{In}(\text{benzyl})_3$ used). Four dark-red plate-like crystals assembled together to form a butterfly pattern.

2. Crystallographic Supplementation

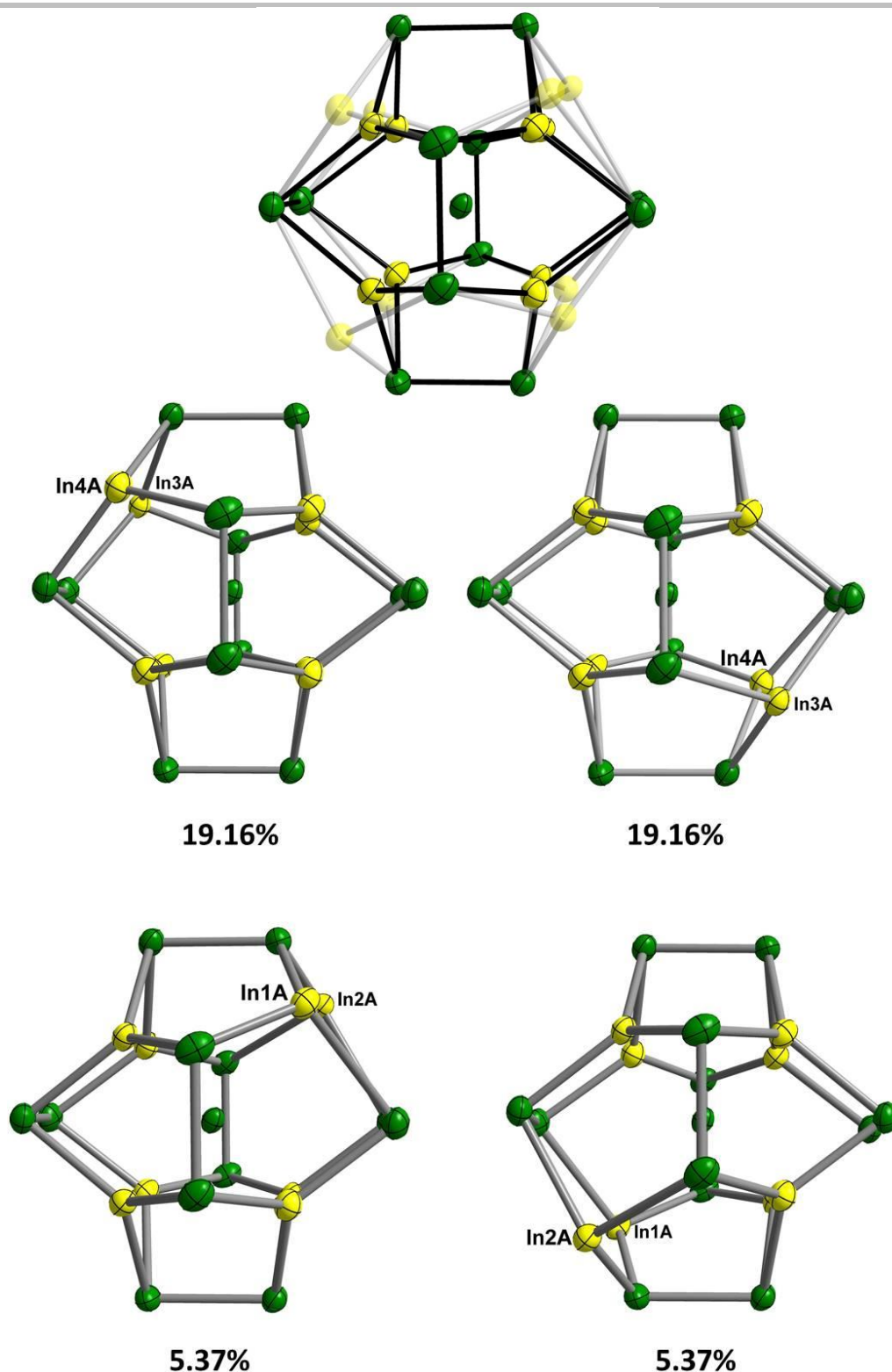
Table S1. X-ray measurements and structure solution of compounds.

Compound	1
Empirical formula	$\text{C}_{772}\text{H}_{144}\text{N}_8\text{O}_{24}\text{K}_4\text{In}_8\text{Sb}_{13}$
Formula weight	4162.16
Crystal system	triclinic
Space group	$P\bar{1}$
$a/\text{\AA}$	15.533(3)
$b/\text{\AA}$	15.882(3)
$c/\text{\AA}$	17.179(3)
$\alpha/^\circ$	111.040(3)
$\beta/^\circ$	115.984(3)
$\gamma/^\circ$	96.795(3)
V	3358.2(10)
Z	2
$\rho_{\text{calc}}/\text{g}\cdot\text{cm}^{-3}$	2.059
$\mu(\text{MoK}\alpha)/\text{mm}^{-1}$	4.084
$F(000)$	1955.0
$2\theta \text{ range}/^\circ$	2.908 to 52.072
Reflections collected / unique	20595 / 13080
Data / restraints / parameters	13080/53/599
R_1/wR_2 ($I > 2\sigma(I)$) ^a	0.0693/ 0.1506
R_1/wR_2 (all data)	0.1481/ 0.1837
GooF (all data) ^b	0.837
Data completeness	0.996
Max. peak/hole $/\text{e}^- \cdot \text{\AA}^{-3}$	2.46/-1.48

Table S2. Selected interatomic distances (in Å) of the experimental and optimized structures of the clusters at the PBE0/Def2-TZVP level of theory.

	Experimental	T_h -[Sb@In ₈ Sb ₁₂] ³⁻	C_{3v} -[Sb@In ₈ Sb ₁₂] ⁵⁻	C_s -[Sb@In ₈ Sb ₁₂] ⁵⁻
				
Sb1-Sb2	2.847(12)	2.8436	2.8542	2.8218
Sb3-Sb4	2.816(16)	2.8436	2.8542	2.8511
Sb5-Sb6	2.812(14)	2.8436	2.8542	2.8891
In1-Sb1	2.838(15)	2.8627	2.8795	3.0266
In1-Sb3'	2.807(12)	2.8627	2.9510	3.0209
In1-Sb6	2.799(6)	2.8627	2.8330	2.9350
In2-Sb5	2.847(16)	2.8627	2.8795	2.8804
In2-Sb4	2.836(16)	2.8627	2.8330	2.8576
In2-Sb1'	2.837(13)	2.8627	2.9510	2.9204
In3-Sb2	2.848(6)	2.8627	2.8923	2.8661
In3-Sb3	2.842(16)	2.8627	2.8330	2.8776
In3-Sb5'	2.857(12)	2.8627	2.9510	2.9053
In4-Sb2	2.822(15)	2.8627	3.1439	3.0266
In4-Sb4	2.834(16)	2.8627	3.1439	3.0209
In4-Sb6	2.820(14)	2.8627	3.1439	2.9350
Sb7-In1	3.006(12)	3.0512	3.0091	3.7637
Sb7-In2	2.993(12)	3.0512	3.0091	3.0065
Sb7-In3	2.977(15)	3.0512	3.0091	2.9905
Sb7-In4	2.978(15)	3.0512	4.4925	3.7637
In1-In4	3.436	3.5232	4.3791	4.3042
In1-In2'	3.474	3.5232	3.5268	3.9532
In1-In3'	3.433	3.5232	3.5268	3.9423
In2'-In3	3.457	3.5232	3.5268	3.5423
In2'-In4'	3.449	3.5232	3.4593	3.4403
In3-In4	3.457	3.5232	4.3791	3.9532
Gap		2.9603 eV	1.9217 eV	1.1532 eV

**Figure S1.** [K(2,2,2-crypt)]₄[In₈Sb₁₃] dispersed in silicon oil.



Structural refinement reveals that the thirteen Sb vertexes are well-ordered, whereas eight In vertexes are disordered at two sets of positions. Regardless of the disorder of the cage, it is clear from the data that the dominating components is the puckered T_h -symmetric $[\text{In}_8\text{Sb}_{12}]$ cage. The secondary component of the disordered In atom is pushed out of the cube with the structure of $[\text{In}_8\text{Sb}_{13}]$ dodecahedron cage reminiscent of the Sb_{20} cage in the $[\text{Sb}@\text{M}_{12}@\text{Sb}_{20}]^{3-}$ cluster. The four orientation occupation ratios of the 5-structure, that with two adjacent In atoms to be placed on these positions, are 0.0537, 0.0537, 0.1916 and 0.1916, respectively, so that the total occupancy of the 5- structure is 0.492, the remaining 0.508 is occupied by 3- structure. The 3-/5- ratio is 51% : 49%, nearly an ideal 1:1 ratio.

Figure S2. Disorder model illustrated by superposition of both compositions.

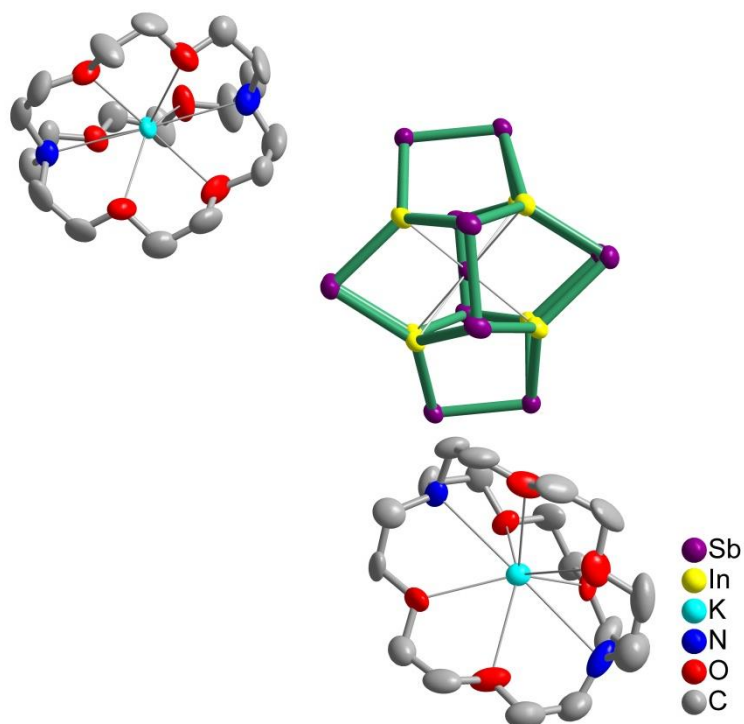


Figure S3. Asymmetric unit of 1 with the cluster fragment. Thermal ellipsoids are drawn at 50% probability. The minor components are omitted for clarity.

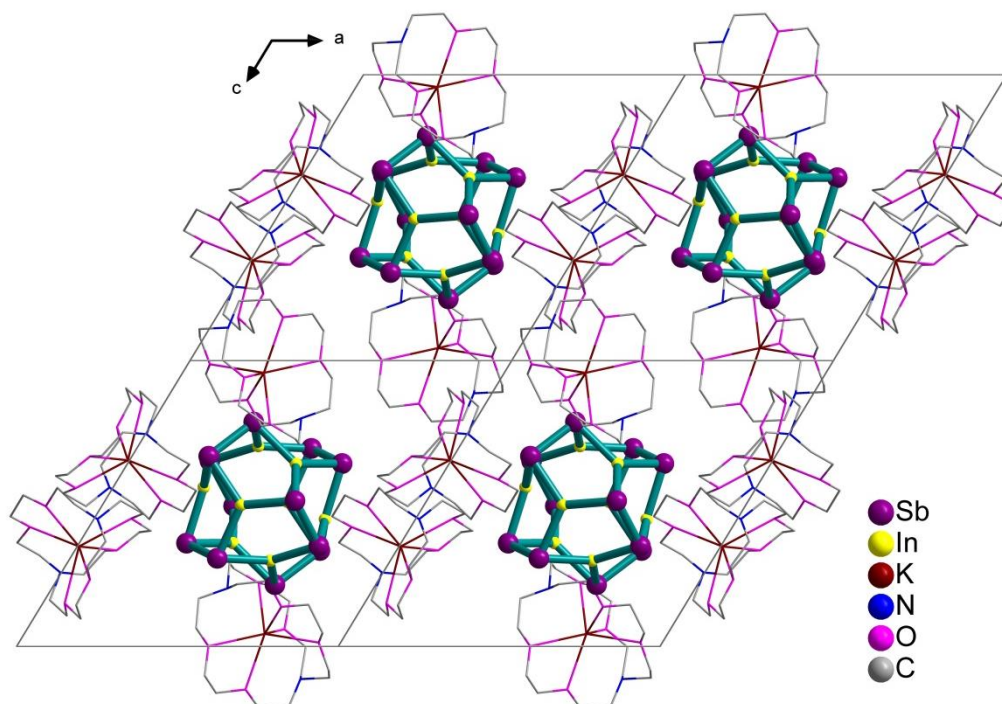


Figure S4. Unit cell of compound 1. Ethylenediamine molecules and minor component in the cluster site are omitted for clarity.

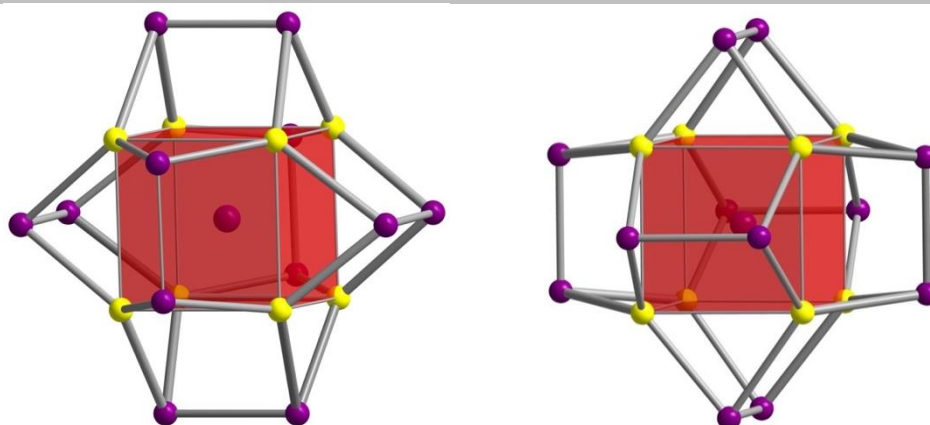


Figure S5. Schematic drawings of the $[\text{Sb}@\text{In}_8\text{Sb}_{12}]^{3-}$ in two perpendicular views, with the $[\text{Sb}@\text{In}_8]$ cubic highlighted in the polyhedral form.

3. Energy Dispersive X-ray (EDX) Spectroscopic Analysis

EDX analysis on **1** (Figure S6) was performed using a scanning electron microscope (Hitachi S-4800) equipped with a Bruker AXS XFlash detector 4010. Data acquisition was performed with an acceleration voltage of 20 kV and an accumulation time of 150 s. The atomic ratio of In/Sb is 8:12.79, which is in good agreement with the experimental crystallographic data.

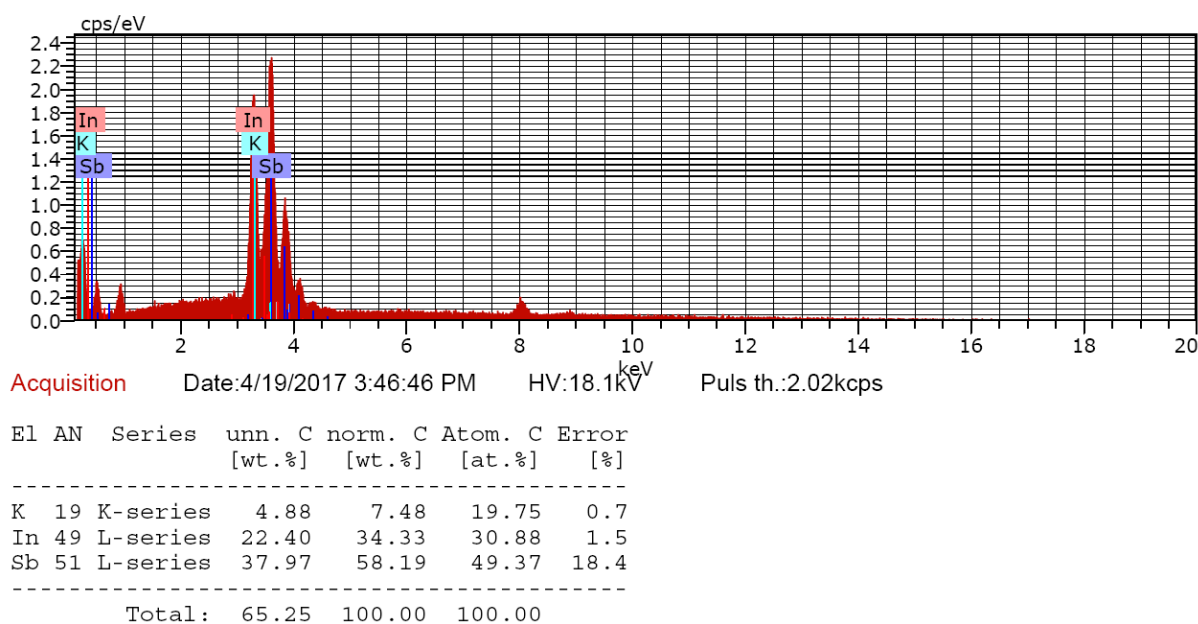


Figure S6. EDX analysis of **1** (K, In, Sb).

4. Electrospray Ionization Mass Spectrometry (ESI-MS)

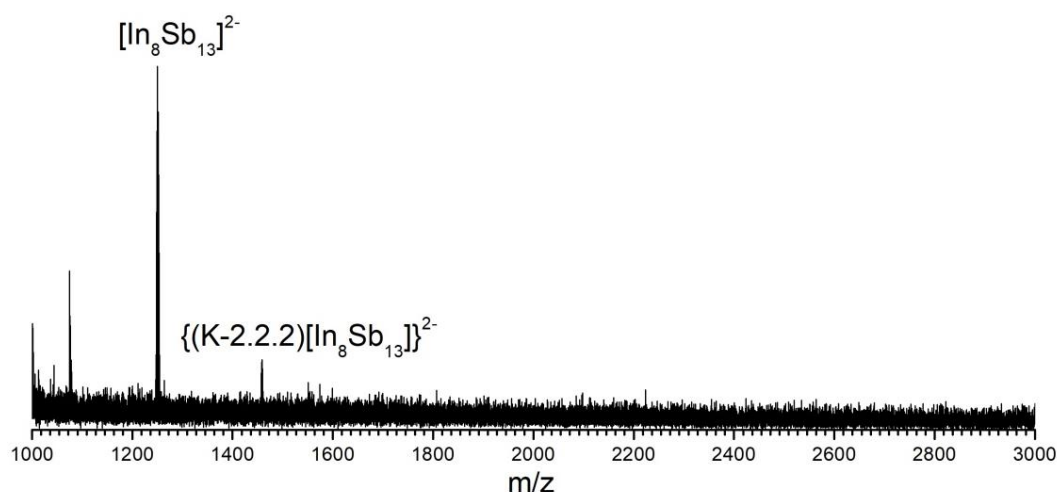


Figure S7. Full negative ion mode spectrum of a DMF solution of a crystalline sample of **1**.

5. Computational Methods and Details

Geometry optimization and frequency calculations were performed using Gaussian 09 software package.⁵ Optimized geometries, total energies are reported at the PBE0/Def2-TZVP⁶ level of theory. The DFT wave functions were found to be stable, so the DFT approximation is valid. To understand the chemical bonding of $[\text{Sb}@\text{In}_8\text{Sb}_{12}]^{3-/4-/5-}$ species we carried out electron localization analysis at the same level of theory using the AdNDP method as implemented in the AdNDP 2.0 code. Previously, AdNDP was shown to be insensitive to the level of theory or the basis set used.⁷ The ChemCraft 1.8 software was used for molecular orbitals visualization of the AdNDP results.

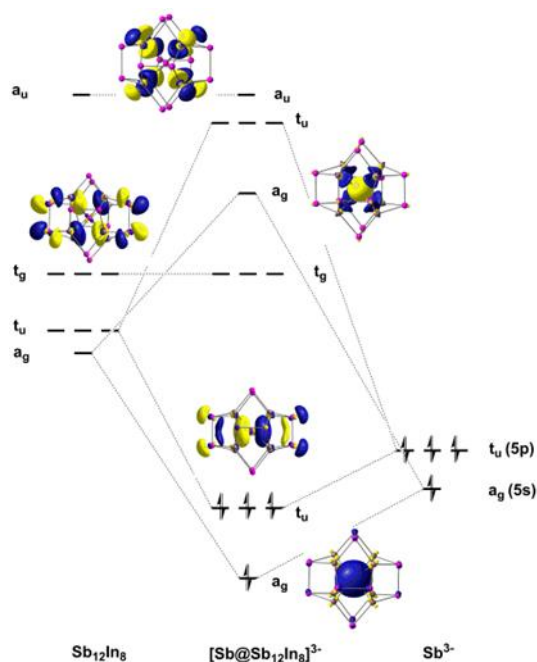


Figure S8. Schematic orbital diagram for $[\text{Sb}@\text{In}_8\text{Sb}_{12}]^{3-}$ cluster, emphasising the interaction of the 5s and 5p orbitals of Sb7 with the formally vacant 5p orbitals on In.

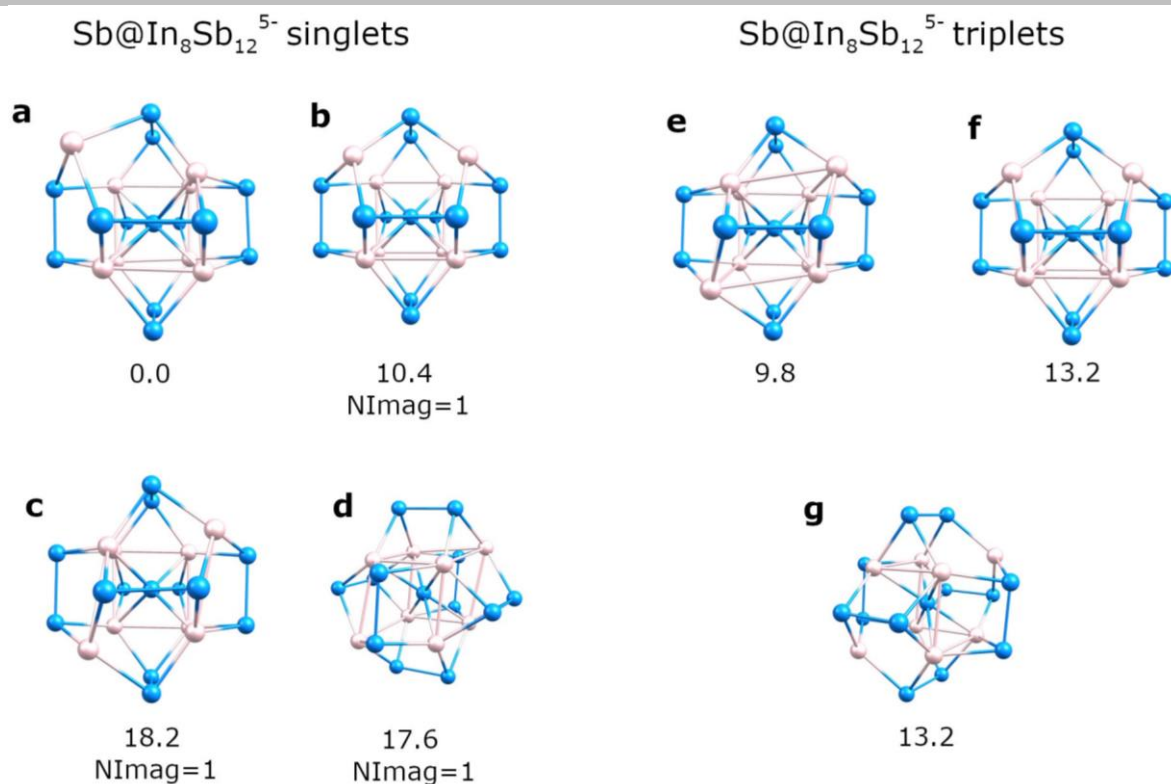


Figure S9. Relative energies (in kcal/mol) of the $[\text{Sb@In}_8\text{Sb}_{12}]^{5-}$ isomers calculated at the PBE0/Def2-TZVP level of theory. Triplet states are 9.8–13.2 kcal/mol higher in energy and correspond to the structures with the T_h -like geometries though with two In atoms pushed out of the In_8 cube. NImag denotes a number of imaginary frequencies.

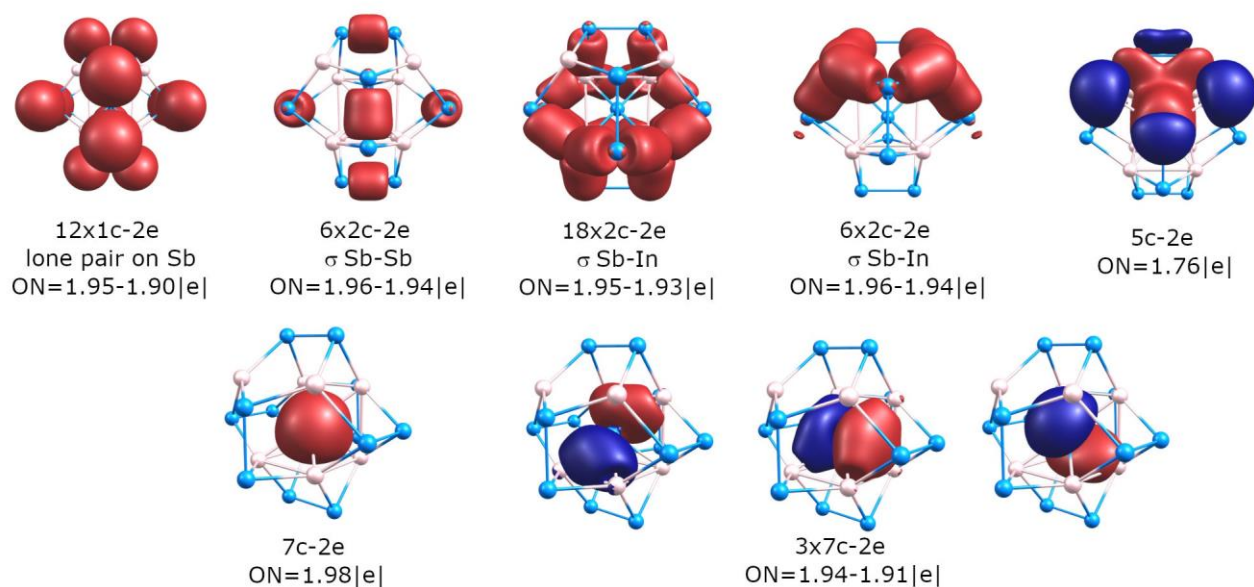


Figure S10. AddNP results of the $[\text{Sb@In}_8\text{Sb}_{12}]^{5-}$ cluster, isomer b.

Table S3. Cartesian coordinates and total electronic energies of the studied clusters.

[Sb@In₈Sb₁₂]³⁻ singlet state	PBE0/Def2-TZVP, E _{total} = -4645.6617185, ZPE = 0.014819			
	49	1.761621000	1.761621000	1.761621000
	49	1.761621000	-1.761621000	1.761621000
	49	-1.761621000	-1.761621000	1.761621000
	49	-1.761621000	1.761621000	1.761621000
	49	1.761621000	1.761621000	-1.761621000
	49	-1.761621000	1.761621000	-1.761621000
	49	-1.761621000	-1.761621000	-1.761621000
	49	1.761621000	-1.761621000	-1.761621000
	51	3.992341000	0.000000000	-1.421808000
	51	3.992341000	0.000000000	1.421808000
	51	-3.992341000	0.000000000	1.421808000
	51	-3.992341000	0.000000000	-1.421808000
	51	1.421808000	3.992341000	0.000000000
	51	-1.421808000	3.992341000	0.000000000
	51	1.421808000	-3.992341000	0.000000000
	51	-1.421808000	-3.992341000	0.000000000
	51	0.000000000	1.421808000	-3.992341000
	51	0.000000000	-1.421808000	-3.992341000
	51	0.000000000	1.421808000	3.992341000
	51	0.000000000	-1.421808000	3.992341000
	51	0.000000000	0.000000000	0.000000000
[Sb@In₈Sb₁₂]³⁻ triplet state	PBE0/Def2-TZVP, E _{total} = -4645.6035904, ZPE = 0.014291			
	49	3.471483000	0.610375000	1.663921000
	49	0.999965000	-2.593037000	1.247260000
	49	-2.158507000	-1.066508000	1.954520000
	49	-0.616124000	2.226501000	2.142324000
	49	2.061326000	1.012423000	-1.857774000
	49	-1.041301000	2.600790000	-1.231893000
	49	-2.627682000	-0.511796000	-1.392044000
	49	0.444680000	-2.119599000	-2.196381000
	51	3.242680000	-1.562033000	-2.235162000
	51	3.706340000	-2.092858000	0.511009000
	51	-3.378106000	1.528351000	2.204150000
	51	-3.764615000	1.980790000	-0.580227000
	51	3.048894000	2.972568000	-0.058021000
	51	0.556498000	4.234800000	0.508431000
	51	-0.643528000	-4.156438000	-0.529066000
	51	-3.148400000	-2.934726000	0.023553000
	51	0.047420000	1.834531000	-3.746390000
	51	-1.293435000	-0.664751000	-3.911700000
	51	1.199415000	0.581632000	3.552917000
	51	-0.121760000	-1.919491000	3.789150000
	51	0.035690000	0.044718000	0.154362000
[Sb@In₈Sb₁₂]⁴⁻ doublet state	PBE0/Def2-TZVP, E _{total} = -4645.4393401, ZPE = 0.016894			
	49	1.786838000	1.786838000	1.786838000
	49	1.786838000	-1.786838000	1.786838000
	49	-1.786838000	-1.786838000	1.786838000
	49	-1.786838000	1.786838000	1.786838000

	49	1.786838000	1.786838000	-1.786838000
	49	-1.786838000	1.786838000	-1.786838000
	49	-1.786838000	-1.786838000	-1.786838000
	49	1.786838000	-1.786838000	-1.786838000
	51	4.034397000	0.000000000	-1.415825000
	51	4.034397000	0.000000000	1.415825000
	51	-4.034397000	0.000000000	1.415825000
	51	-4.034397000	0.000000000	-1.415825000
	51	1.415825000	4.034397000	0.000000000
	51	-1.415825000	4.034397000	0.000000000
	51	1.415825000	-4.034397000	0.000000000
	51	-1.415825000	-4.034397000	0.000000000
	51	0.000000000	1.415825000	-4.034397000
	51	0.000000000	-1.415825000	-4.034397000
	51	0.000000000	1.415825000	4.034397000
	51	0.000000000	-1.415825000	4.034397000
	51	0.000000000	0.000000000	0.000000000
[Sb@In₈Sb₁₂]⁵⁻ singlet state, isomer a	PBE0/Def2-TZVP, E _{total} = -4645.1770612, ZPE = 0.013796			
	49	1.110145000	-0.888534000	-2.722821000
	49	-1.029635000	-2.726406000	-0.605915000
	49	1.110181000	-1.914047000	2.130751000
	49	3.050520000	-0.000295000	-0.000038000
	49	-1.029077000	1.888171000	-2.058205000
	49	1.110775000	2.802173000	0.592007000
	49	-1.029080000	0.838550000	2.664196000
	49	-4.402040000	0.000490000	0.000099000
	51	-3.085007000	0.108264000	-2.852483000
	51	-1.400103000	-2.129877000	-3.398484000
	51	3.261959000	-0.136117000	2.888717000
	51	1.547744000	2.103632000	3.347754000
	51	1.547649000	1.847140000	-3.495914000
	51	3.262239000	2.569259000	-1.326894000
	51	-3.085172000	-2.523948000	1.332933000
	51	-1.399854000	-1.878047000	3.543869000
	51	-1.399154000	4.008389000	-0.145368000
	51	-3.084571000	2.416820000	1.519796000
	51	3.261579000	-2.434236000	-1.562032000
	51	1.546983000	-3.951394000	0.147997000
	51	0.090459000	0.000017000	0.000038000
[Sb@In₈Sb₁₂]⁵⁻ singlet state, isomer b	PBE0/Def2-TZVP, E _{total} = -4645.16025537, ZPE = 0.013496 one imaginary frequency (-74.8264 cm ⁻¹)			
	49	-0.161736000	-2.497453000	1.669865000
	49	2.401338000	-0.204808000	1.771127000
	49	2.401338000	-0.204808000	-1.771127000
	49	-0.161736000	-2.497453000	-1.669865000
	49	-2.439362000	0.186845000	1.746891000
	49	-2.439362000	0.186845000	-1.746891000
	49	0.219235000	3.069487000	-2.152084000
	49	0.219235000	3.069487000	2.152084000
	51	-0.903885000	0.980050000	4.022591000
	51	0.929400000	-1.203480000	4.033163000
	51	0.929400000	-1.203480000	-4.033163000
	51	-0.903885000	0.980050000	-4.022591000
	51	-3.038572000	-2.652805000	1.420987000

	51	-3.038572000	-2.652805000	-1.420987000
	51	3.107206000	2.549530000	1.410898000
	51	3.107206000	2.549530000	-1.410898000
	51	-3.832846000	2.004258000	0.000000000
	51	-1.615047000	3.855880000	0.000000000
	51	1.573762000	-4.120260000	0.000000000
	51	3.648876000	-2.140726000	0.000000000
	51	-0.000467000	-0.010428000	0.000000000
[Sb@In₈Sb₁₂]⁵⁻ singlet state, isomer c	PBE0/Def2-TZVP, E _{total} = -4645.14777538, ZPE = 0.013517 one imaginary frequency (-129.828 cm ⁻¹)			
	49	0.056009000	2.433485000	1.719107000
	49	2.493711000	-0.049886000	1.837682000
	49	-0.056009000	-2.433485000	1.719107000
	49	-2.493711000	0.049886000	1.837682000
	49	0.000000000	3.114971000	-2.143475000
	49	-2.322395000	0.071868000	-1.707792000
	49	0.000000000	-3.114971000	-2.143475000
	49	2.322395000	-0.071868000	-1.707792000
	51	2.880966000	2.741457000	-1.381777000
	51	2.918187000	2.783843000	1.467427000
	51	-2.918187000	-2.783843000	1.467427000
	51	-2.880966000	-2.741457000	-1.381777000
	51	-1.776808000	3.889818000	0.070102000
	51	-3.808313000	1.856546000	0.006927000
	51	3.808313000	-1.856546000	0.006927000
	51	1.776808000	-3.889818000	0.070102000
	51	-0.958821000	1.065580000	-4.008955000
	51	0.958821000	-1.065580000	-4.008955000
	51	-0.986457000	1.041155000	4.085709000
	51	0.986457000	-1.041155000	4.085709000
	51	0.000000000	0.000000000	0.086994000
[Sb@In₈Sb₁₂]⁵⁻ singlet state, isomer d	PBE0/Def2-TZVP, E _{total} = -4645.14871644, ZPE = 0.013420 one imaginary frequency (-109.5444 cm ⁻¹)			
	49	2.964321000	0.145682000	0.039905000
	49	1.029038000	-2.778256000	-0.179854000
	49	-0.853329000	-1.425064000	2.459980000
	49	1.266772000	1.754576000	3.137133000
	49	0.853329000	1.425064000	-2.459980000
	49	-1.029038000	2.778256000	0.179854000
	49	-2.964321000	-0.145682000	-0.039905000
	49	-1.266772000	-1.754576000	-3.137133000
	51	1.488718000	-0.953827000	-3.915883000
	51	3.200349000	-2.036347000	-1.898907000
	51	-1.488718000	0.953827000	3.915883000
	51	-3.200349000	2.036347000	1.898907000
	51	3.010959000	2.802263000	-1.037436000
	51	1.442113000	3.899061000	1.085209000
	51	-1.442113000	-3.899061000	-1.085209000
	51	-3.010959000	-2.802263000	1.037436000
	51	-1.622063000	2.853838000	-2.686889000
	51	-3.205002000	0.477814000	-2.821258000
	51	3.205002000	-0.477814000	2.821258000
	51	1.622063000	-2.853838000	2.686889000
	51	0.000000000	0.000000000	0.000000000
[Sb@In₈Sb₁₂]⁵⁻ triplet state, isomer e	PBE0/Def2-TZVP, E _{total} = -4645.1615402, ZPE = 0.013818			

	49	0.026003000	1.700800000	2.361343000
	49	3.170472000	2.171439000	-0.010296000
	49	2.420017000	-1.683413000	-0.023898000
	49	0.002162000	-1.834562000	2.489698000
	49	-3.169279000	2.172227000	0.011341000
	49	-2.421472000	-1.680809000	0.022533000
	49	-0.002092000	-1.833227000	-2.490838000
	49	-0.025645000	1.703059000	-2.359424000
	51	-1.029872000	3.984444000	-0.987730000
	51	1.031247000	3.983262000	0.992070000
	51	1.037569000	-4.064305000	0.980889000
	51	-1.040513000	-4.062458000	-0.983847000
	51	-2.793510000	1.358061000	2.842624000
	51	-2.845574000	-1.500021000	2.872241000
	51	2.793725000	1.359727000	-2.841835000
	51	2.845422000	-1.498192000	-2.873292000
	51	-3.871723000	-0.056655000	-1.835694000
	51	-1.826105000	-0.038473000	-3.827909000
	51	1.827531000	-0.041918000	3.827660000
	51	3.871615000	-0.060561000	1.834197000
	51	0.000030000	-0.050365000	0.000184000
[Sb@In₈Sb₁₂]⁵⁻ triplet state, isomer f	PBE0/Def2-TZVP, E _{total} = -4645.159024, ZPE = 0.013720			
	49	0.131264000	1.783476000	-2.418005000
	49	-2.486904000	1.675952000	-0.155029000
	49	-2.486968000	-1.675834000	-0.154967000
	49	0.131158000	-1.783584000	-2.417942000
	49	3.026193000	2.201831000	0.160248000
	49	3.026085000	-2.201937000	0.160358000
	49	-0.177362000	-1.743524000	2.438793000
	49	-0.177270000	1.743622000	2.438725000
	51	0.849147000	4.024723000	1.050598000
	51	-1.061732000	4.031962000	-1.068928000
	51	-1.061931000	-4.031965000	-1.068761000
	51	0.848969000	-4.024718000	1.050748000
	51	2.954765000	1.439764000	-2.667343000
	51	2.954684000	-1.440049000	-2.667277000
	51	-3.064771000	1.429551000	2.670491000
	51	-3.064849000	-1.429299000	2.670542000
	51	3.628429000	-0.000030000	2.021553000
	51	1.541797000	0.000039000	3.959001000
	51	-1.626156000	-0.000030000	-3.904849000
	51	-3.841269000	0.000048000	-2.097318000
	51	-0.004603000	0.000002000	0.001408000
[Sb@In₈Sb₁₂]⁵⁻ triplet state, isomer g	PBE0/Def2-TZVP, E _{total} = -4645.1558281, ZPE = 0.013645			
	49	-1.082920000	-0.932357000	-2.615384000
	49	-3.854029000	-0.000465000	0.000440000
	49	-1.081851000	-1.799242000	2.115276000
	49	1.082845000	-2.730972000	-0.500490000
	49	1.081874000	1.798893000	-2.114973000
	49	3.854332000	0.000340000	-0.000594000
	49	1.082637000	0.932350000	2.615165000
	49	-1.082785000	2.731363000	0.500641000

	51	-1.446925000	3.264781000	-2.295531000
	51	-3.160213000	1.022438000	-2.718240000
	51	1.447176000	-3.264739000	2.295576000
	51	3.160169000	-1.022112000	2.718072000
	51	1.445682000	-0.355583000	-3.975471000
	51	3.159494000	-1.842733000	-2.245429000
	51	-3.159511000	1.842697000	2.245353000
	51	-1.445775000	0.355563000	3.975470000
	51	3.159276000	2.865971000	-0.474170000
	51	1.446260000	3.620817000	1.679437000
	51	-1.446081000	-3.620802000	-1.679369000
	51	-3.159213000	-2.866158000	0.474224000
	51	-0.000440000	-0.000053000	0.000001000
[Sb@In₈Sb₁₂]⁵⁻ T_h triplet state	PBE0/Def2-TZVP, E _{total} = -4645.1349649, ZPE = 0.012210, three imaginary frequencies (-135.0209 cm ⁻¹ T _u)			
	49	1.810043000	1.810043000	1.810043000
	49	1.810043000	-1.810043000	1.810043000
	49	-1.810043000	-1.810043000	1.810043000
	49	-1.810043000	1.810043000	1.810043000
	49	1.810043000	1.810043000	-1.810043000
	49	-1.810043000	1.810043000	-1.810043000
	49	-1.810043000	-1.810043000	-1.810043000
	49	1.810043000	-1.810043000	-1.810043000
	51	4.083850000	0.000000000	-1.412733000
	51	4.083850000	0.000000000	1.412733000
	51	-4.083850000	0.000000000	1.412733000
	51	-4.083850000	0.000000000	-1.412733000
	51	1.412733000	4.083850000	0.000000000
	51	-1.412733000	4.083850000	0.000000000
	51	1.412733000	-4.083850000	0.000000000
	51	-1.412733000	-4.083850000	0.000000000
	51	0.000000000	1.412733000	-4.083850000
	51	0.000000000	-1.412733000	-4.083850000
	51	0.000000000	1.412733000	4.083850000
	51	0.000000000	-1.412733000	4.083850000
	51	0.000000000	0.000000000	0.000000000

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