Electronic Supplementary Information for Dalton Transactions

SUPPORTING INFORMATION

Metastable Se_6 as a Ligand for Ag^+: from Isolated Molecular to Polymeric 1D and 2D Structures

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*To whom correspondence should be addressed: Jörn Schmedt auf der Günne ($^{109}Ag/^{19}F$ NMR), Ingo Krossing (theoretical calculations and isolated $[(OSO)_xAgSe_6Ag(OSO)_x]^{2+}$ (x = 1, 2) preparation), and Jack Passmore (problem conception and the remainder of preparations and structures).

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S1 Reactions leading to **3** and **4**

Table S1.1 Reaction data (g, mmol) of some reactions

Code	Reaction	Mole ratio[a]	Time and temperature	Emperical formula based on weight changes[b]	Emperical formula based on chemical analysis	Single crystal X-ray (SCX) and X-ray powder diffraction (XRD)
a	$AgAsF_6$ + Se powder	10 : 1	several minutes, r.t.			**3** (SCX)
b	$AgAsF_6$ + Se pellets	2 : 1	2d, r.t.	$Se_{2.7}AgAsF_6$	$Se_{2.90}AgAs_{1.02}F_{5.95}$	**3** (XRD)
c	$AgAsF_6$ + Se pellets	1 : 8[c]	24d, 5°C	$Se_{3.0}AgAsF_6$	$Se_{3.05}AgAs_{1.02}F_{6.12}$	
d	$Se_4(AsF_6)_2$+2Ag+2Se	1 : 2 : 2	15d, r.t.	Se_3AgAsF_6	$Se_{2.74}AgAs_{0.96}F_{5.65}$	**3** (XRD)
e	$AgSbF_6$ + Se powder	20 : 1	several minutes, r.t.			**2** (SCX)
f	$AgSbF_6$ + Se powder	3 : 2	14d, r.t.	$Se_{2.2}AgSbF_6$		**?** (XRD)
g	$AgSbF_6$ + Se powder	1 : 3	2d, r.t.	$Se_{3.4}AgSbF_6$		
h	$AgSbF_6$ + Se pellets	1 : 8.5[c]	24d, 5 °C	$Se_{4.6}AgSbF_6$	$Se_{5.4}AgSb_{1.07}F_{6.17}$	**?** (XRD)

a) Weight given in Table S1.2;
b) Based on the amount of the Se and $AgMF_6$ consumed;
c) All $AgMF_6$ consumed in this reaction;
d) The insoluble product and unreacted $AgSbF_6$ were not separated.

Table S1.2

code	Reactions	$AgMF_6$ (M=As, Sb)	Se (powder or pellets)	$AgMF_6$ consumed	Se consumed	Se : $AgMF_6$[a]
b	$AgAsF_6$ + Se powder	1.315, 4.431	0.164, 2.077	0.05, 0.168	0.036, 0.456	2.7 : 1
c	$AgAsF_6$ + Se pellets	0.934, 3.147	1.965, 24.886	0.934, 3.147	0.755, 9.562	3.0 : 1
f	$AgSbF_6$ + Se powder	3.000, 8.730	0.443, 5.610	0.870, 2.532	0.443, 5.610	2.2 : 1
g	$AgSbF_6$ + Se powder	1.111, 3.233	0.685, 8.675	0.871, 2.535	0.685, 8.675	3.4 : 1
h	$AgSbF_6$ + Se pellets	2.055, 5.980	4.011, 50.798	2.055, 5.980	2.166, 27.431	4.6 : 1

a) The mole ratio (Se : $AgMF_6$) is based on the amount of the consumed Se and consumed $AgMF_6$.

Table S1.3

Comparison of Raman and IR frequencies of the insoluble products from reaction b, c, d (see Tables S1.1 and S1.2), Se_6 (s),[a] Se_6 in SiO_2 matrix,[b] Se powder,[a] Se pellets,[a] and AsF_6^- (in O_2AsF_6)[c] with relative peak intensities in parentheses.[d]

Se_6 (s)	Se powder	Se_6 in SiO_2 matrix	Se pellets	b (Ra)	b(IR)	c (Ra)	c(IR)	d(Ra)	d(IR)	AsF_6^- (Ra)	AsF_6^- (IR)	Assign.[e]
				712(1) 691(1)	698(10)	712(0.5)	704(10)	709(0.5)	703(10)		700(10)	$\nu_3(AsF_6^-)$, F_u
				673(5)		673(3)		672(2)		689(10)		$\nu_1(AsF_6^-)$, A_g
					666(8)	639(0.2)	666(8)		667(8)			?
				574(0.5)						573(5)		$\nu_2(AsF_6^-)$, E_g
					561(3)				563(3)			
				558(0.5)				491(0.5)				?
						401(0.3)					385(1)	$\nu_4(AsF_6^-)$, F_u
					398(1)				397(1)			
				401(0.5)	385(2)	373(1)		372(1)	388(2)	375(1)		$\nu_5(AsF_6^-)$, F_g
247(10)		276(9)	251(9.5)			270(10)		270(10)				ν(SeSe), A_{1g}
	236(10)	263(2)	235(10)	373(3)		256(7)		254(7)				ν(SeSe), E_g
221(1)						170(5)		169(5)				ν_s(SeAgSe)
				272(10)		156(3)						?
	144(0.5)		146(1)									δ(SeSeSe)
		133(2)	133(1)	256(5)				123(5)				δ(SeSeSe), A_{1g}
129(3)		102(10)	111(1)	171(9)		116(7)		115(4)				
102(2)			99(0.5)									δ(SeSeSe), E_g
				126(6)								
				113(5)								

a) Based on Raman spectra of this work, Se powder consists of trigonal Se_∞ and Se pellets are a mixture of Se_∞ and Se_6. K. Nagata, K. Ishibashi, Y. Miyamoto, *Jpn. J. Appl. Phys.* **1981**, *20*, 463; b) A micro porous pure SiO_2 modification consisting of pseudohexagonal sheets of pentagondodecahedral cages, stacked in an ABCABC sequence and interconnected by O-Si-O bridges. G. Wirnsberger, H. P. Fritzer, R. Zink, A. Popitsch, B. Pillep, P. Behrens, *J. Phys. Chem. B*, **1999**, *103*, 5797; c) C. Naulin, R. Bougon, *J. Chem. Phys.*, **1976**, *64*, 4156; d) Peak intensities were determined by estimating the area (for Raman) and height (for IR) of peaks; and e) The AsF_6^- assignments are based on ideal O_h symmetry and for Se_6 on ideal D_{3d} symmetry.

Table S1.4

Comparison of Raman frequencies of the insoluble products from reaction f, g, and h (see Table S1.1 and S1.2), together with Se_6,[a] Se powder[a] and Se pellets[a]

Se_6	Se powder	Se pellets	g	f	h	Assign.[b]
			650(0.5)	644(1)		$\nu_1(SbF_6^-)$, A_g
			518(0.1)	513(0.2)		$\nu_2(SbF_6^-)$, E_g
				298(0.8)		$\nu_5(SbF_6^-)$, F_g
247(10)		251(9.5)	272(2)	271(1)	271(5) 261(10)	ν(SeSe), A_{1g}
221(1)	236(10)	235(10)	253(10)	253(10)	253(8)	ν(SeSe), E_g
			161(4)	161(2)		ν_s(SeAgSe)
129(3)	144(0.5)	146(1) 133(1)	124(1)		147(3) 134(6)	δ(SeSeSe), A_{1g}
102(2)		111(1) 99(0.5)	97(5)	97(2)	105(5)	δ(SeSeSe), E_g

a) Based on Raman spectra of this work, Se powder consists of trigonal Se_∞ and Se pellets are a mixture of Se_∞ and Se_6. K. Nagata, T. Ishibashi, Y. Miyamoto, *Jpn. J. Appl. Phys.* **1981**, *20*, 463; b) Peak intensities were determined by estimating the area (for Raman) and height (for IR) of peaks. The AsF_6^- assignments are based on ideal O_h symmetry and for Se_6 on ideal D_{3d} symmetry.

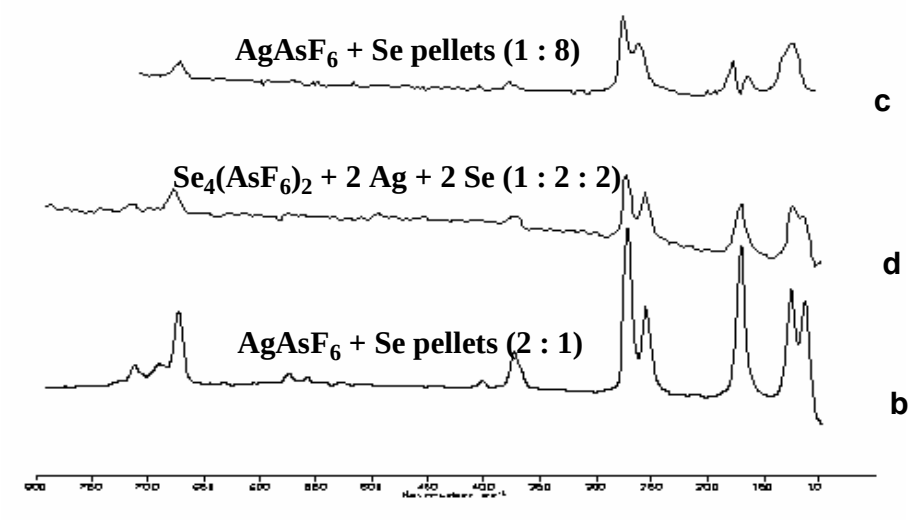


Figure S1.5 FT-Raman spectrum of the yellow insoluble product from Reaction b, c, and d. Experimental parameters: b. 1200 scans, 4 cm^{-1}, r.t.; c and d. 1000 scans, 4 cm^{-1}, r.t..

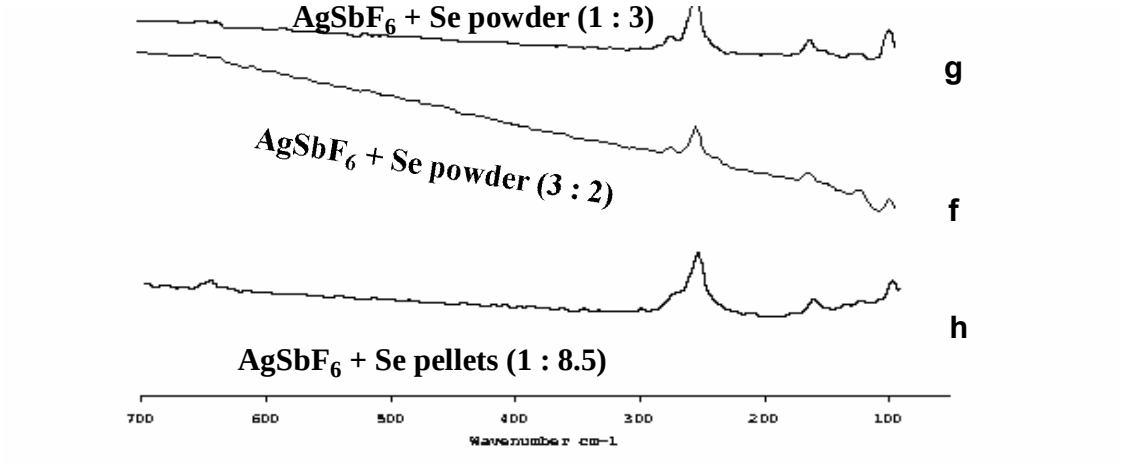


Figure S1.6 FT-Raman spectrum of the yellow insoluble product from reaction f, g and h (**g.** 2000 scans, 4 cm^{-1}, r.t.; **f.** 5 mm NMR tube, 2000 scans, 4 cm^{-1}, r.t.; **h .** 1000 scans, 4 cm^{-1}, r.t.).

Table S 1.7: ^{109}Ag and ^{19}F solid NMR

code	Reactions (mole ratio)	Compound	δiso^{109}Ag (ppm)	δiso^{19}F (ppm)	T_1 (^{19}F, s)
		AgF	-47	-318.2	~200
		AgF_2	-189	-199.5	
		$AgSbF_6$	-221	-127.7	~0.3
		$AgAsF_6$	-243	-63 ~ -71~ -79	
		AgI_2SbF_6	119	-97 ~ -124, sextet	~3
		AgI_2AsF_6	112	-50 ~ -57, quartet	~10
b	$AgAsF_6$ + Se pellets (2 : 1)	**3**	-42, -220	-52 ~ -59, quartet	~2
f	$AgSbF_6$ + Se powder (3 : 2)	**2** ? or $Se_6Ag_2(SbF_6)_2$?	359s, 86s, -335	-95 ~ -140	~1
h	$AgSbF_6$ + Se pellets (1 : 8.5)	Se_6AgSbF_6 ?	483, 429, 113, -292s	-104, -114, doublet	~1

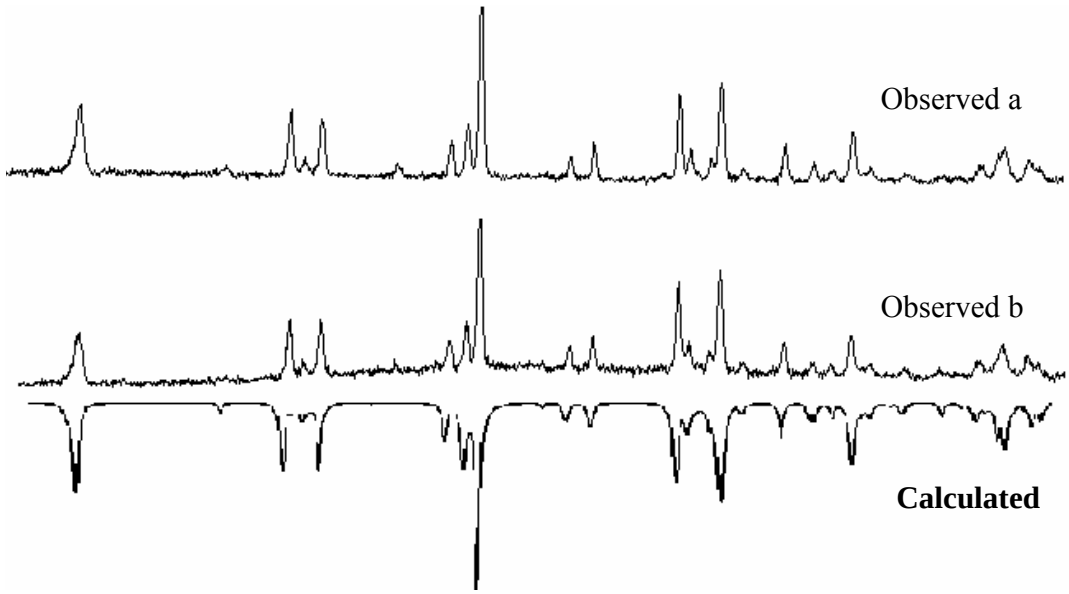


Figure S1.8: X-ray powder diffraction patterns. Observed a: XRD of the yellow insoluble product from the reaction Se pellets + $AgAsF_6$; observed b: XRD of the yellow insoluble product from the reaction 2Se + 2Ag + $Se_4(AsF_6)_2$; Calculated: XRD calculated from crystal structure of **4**

S 2 Detailed description of the X-ray single crystal structures:

S 2.1 Crystal structure of **1**

1: A single crystal X-ray structure determination showed that **1** contains discrete $[(OSO)AgSe_6Ag(OSO)]^{2+}$ dications (Fig. 1a in paper) and $[Sb(OTeF_5)_6]^-$ anions packed in a TiO_2 type structure with a cubic close packed $[Sb(OTeF_5)_6]^-$ anion and every second octahedral hole filled by $[(OSO)AgSe_6Ag(OSO)]^{2+}$ in agreement with the radius ratio rule. The very large spherical $[Sb(OTeF_5)_6]^-$ anions [outer diameter: 10.677 + 2 $r_{cov.}$(F) = 12.117 Å] form a cubic close packed lattice where the cations occupy every second octahedral hole. The anions are surrounded trigonally by three cations and the cations octahedrally by six anions (see graphic representations in Figure S2.1.1). Neglecting the coordinated SO_2 molecules (which will distort the almost spherical $Ag_2Se_6^{2+}$ cation to an ellipsoid) a cation diameter of 7.328 Å is found [outer diameter 5.048 + 2 $r_{ion.}$(Ag) = 7.328 Å] giving a ratio $r_{cat.}/r_{anion}$ of 0.605. This is in agreement with a Rutile Ti structure which requires a ratio $r_{cat.}/r_{anion}$ between 0.414 and 0.737. This supports the thesis that the large anions and cations of this kind are highly ionic .

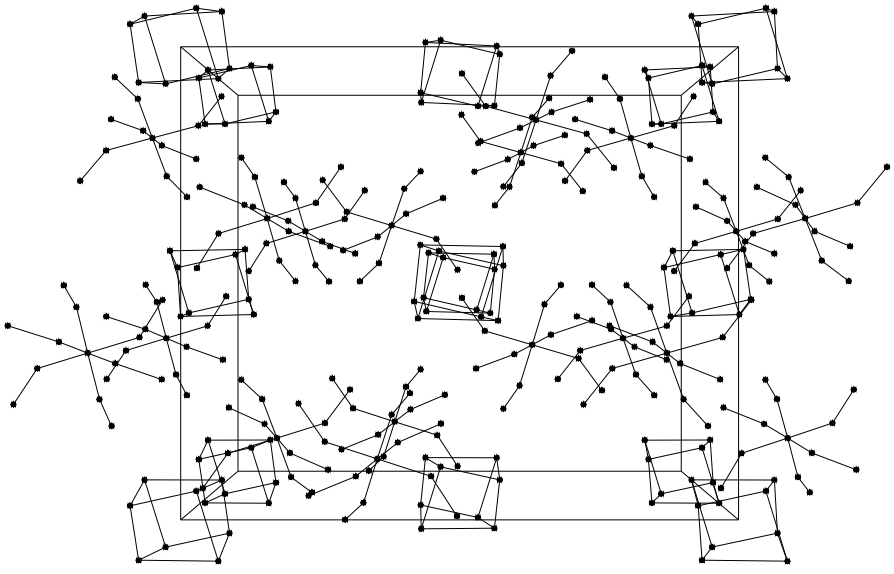


Figure S2.1.1: Representation of the unit cell in **1**. The cations form a cubic face centred packing. All fluorine atoms and the SO_2 molecules are omitted for clarity.

The $[(OSO)AgSe_6Ag(OSO)]^{2+}$ dication contains a D_{3d} symmetric, $[Ag_2Se_6]^{2+}$ heterocubane and two disordered SO_2 molecules which each coordinate to one silver atom. The structure is derived from a six-

membered Se_6 ring in the chair conformation with a very similar geometry to that of Se_6 (Table 1, Figure 1 in main text). The selenium atoms in Se_6 coordinate alternatively to one of the two silver atoms above or below the ring plane (Ag-Se 2.885(2) Å). The geometry of $[(OSO)AgSe_6Ag(OSO)]^{2+}$ is similar to that of $[Nb_2Sn_6(C_6H_5Me_2)_2]^{2-}$(S2.1.2).[1]

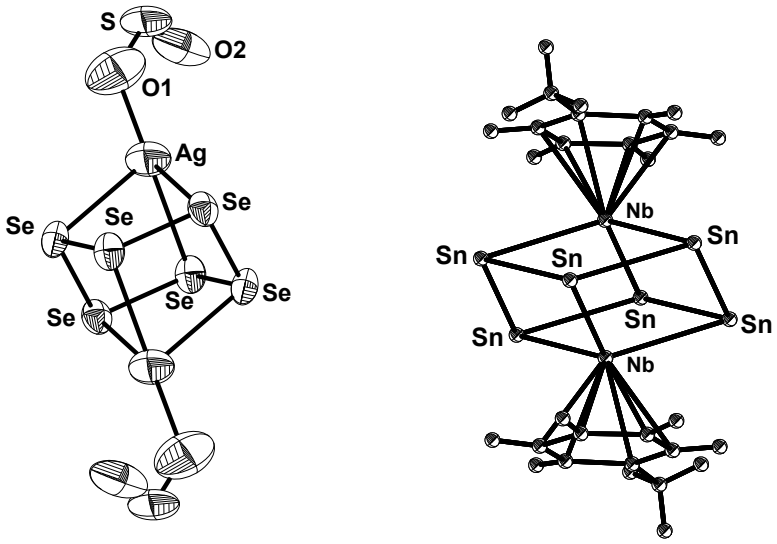


Figure S2.1.2: Comparison of $[(OSO)AgSe_6Ag(OSO)]^{2+}$ and $[Nb_2Sn_6(C_6H_5Me_2)_2]_2^{-}$ geometries. Thermal ellipsoids are drawn at the 50 % probability level.

There are also similarities between the solid state structures of the $Se_6I_2^{2+}$ dication and the $[Ag_2Se_6]^{2+}$ framework in the $[(OSO)AgSe_6Ag(OSO)]^{2+}$ dication (Fig. S2.1.3). One localised, strong Se-I bond and two weaker Se--I contacts in $Se_6I_2^{2+}$ are exchanged for three equal Se-Ag bonds in $[Ag_2Se_6]^{2+}$.

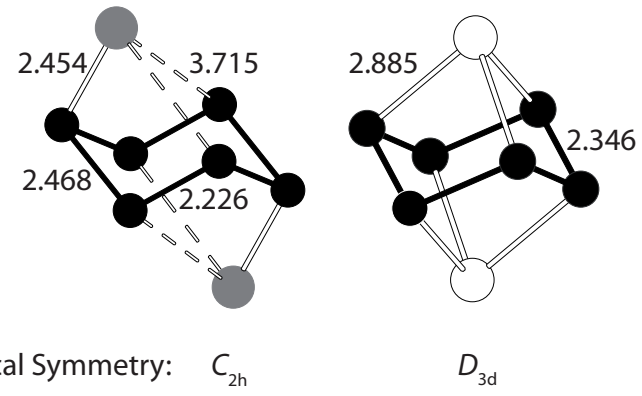


Figure S2.1.3: Comparison of the $Se_6I_2^{2+}$ and "$Se_6Ag_2^{2+}$" geometries in the solid state.

Each selenium atom has three contacts to fluorine atoms at 3.170(7), 3.384(7), and 3.435(7) Å, which are below or near the sum of their Van der Waals radii (3.40 Å) (Fig. S2.1.4). All other contacts are

greater than 3.680 Å. These Se--F contacts are longer than those found in the salts $Se_4(Sb_4F_{17})(SbF_6)$ (2.69 to 3.37 Å)[2] and $Se_3X_3(AsF_6)$[3, 4] (X = Cl 2.688 to 3.414 Å, Br 2.79 to 3.22 Å).

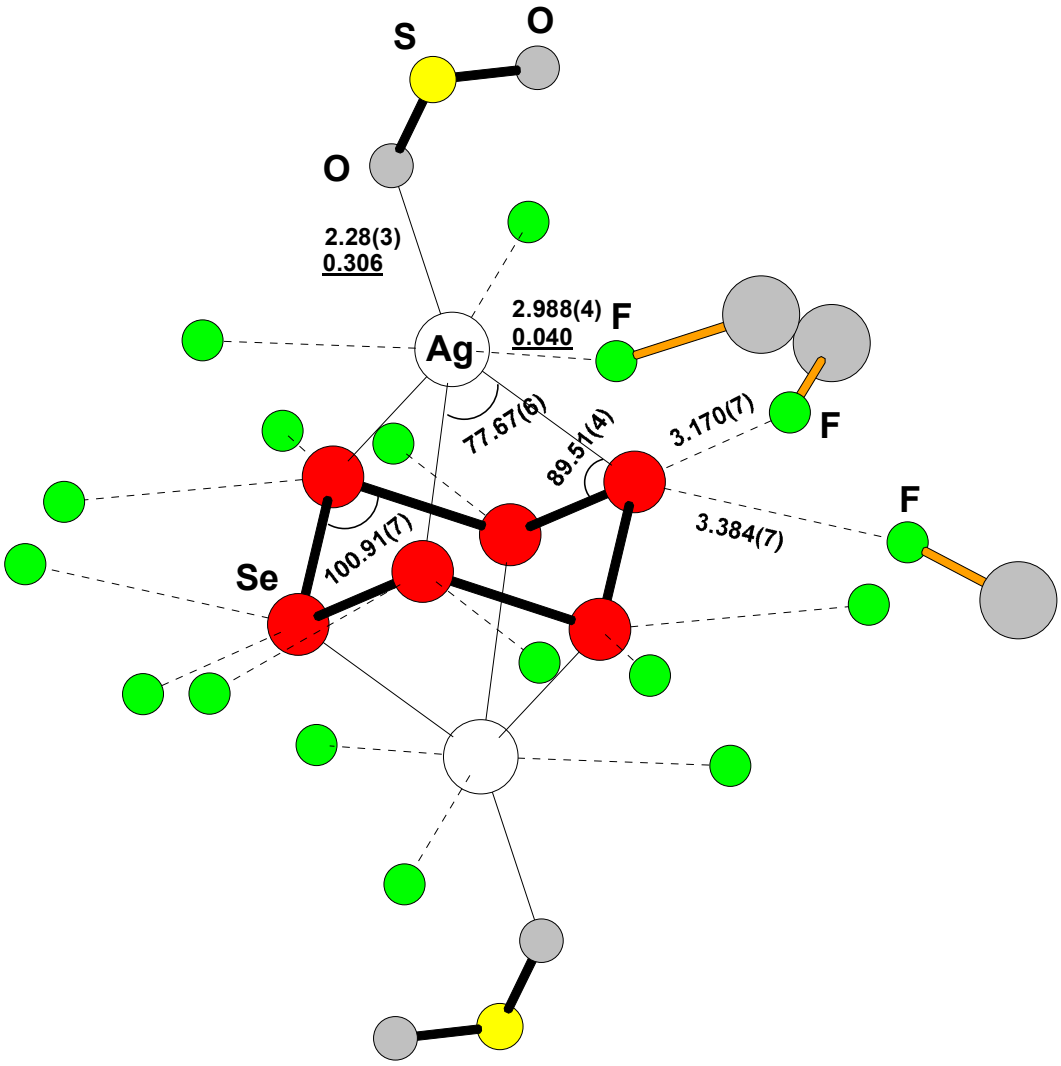


Figure S2.1.4: Coordination sphere of "Se_6Ag_2" in **1** including one of the three disordered SO_2 molecules

Each silver atom in the $[(OSO)AgSe_6Ag(OSO)]^{2+}$ dication is coordinated to one SO_2 molecule, with a threefold axes incorporating all sulphur and silver atoms passing through the cation, and the SO_2 molecules rotationally disordered around the threefold axes such that the required site symmetry (D_{3d}) is maintained. All three equivalent positions were found for each oxygen atom (S2.1.5).

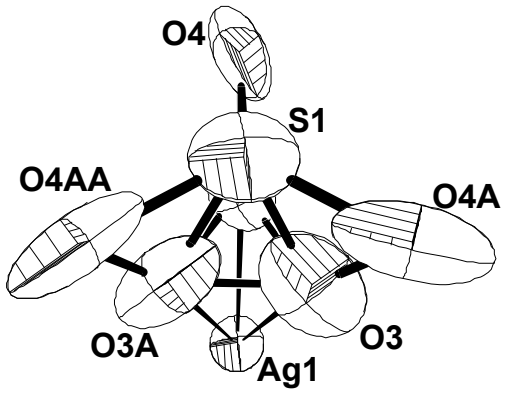
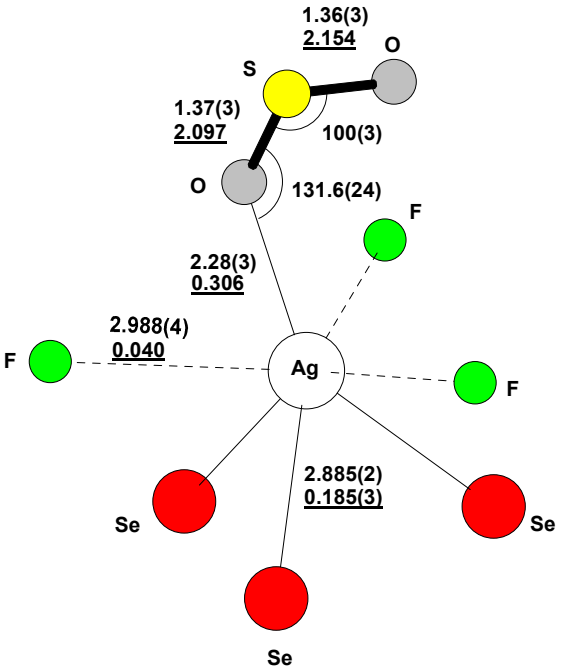
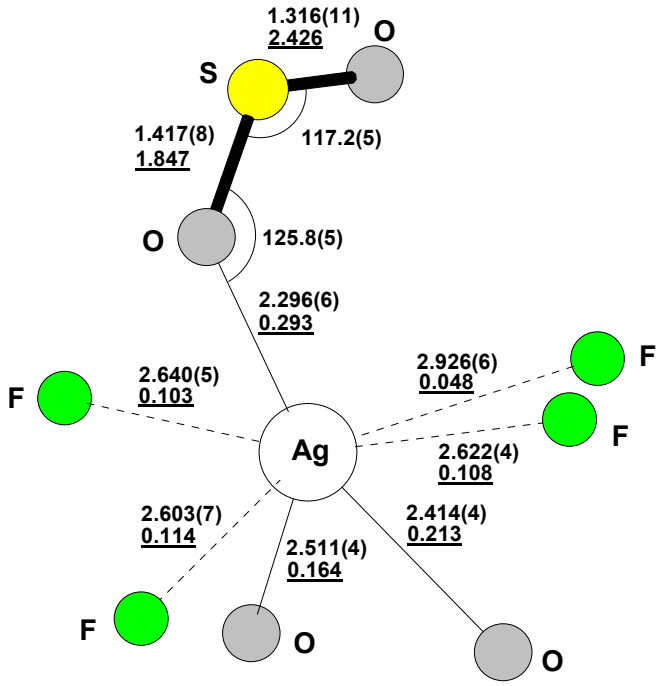


Figure S2.1.5: Threefold rotational disorder of the SO_2 molecule in 1 lying on the threefold axes running through the S-Ag-Ag-S vector as represented by one $Ag(SO_2)$ unit. The thermal ellipsoid are drawn at the 25% probability level.

Correspondingly the standard deviations of the S-O [1.36(3) and 1.37(3) Å] and Ag-O [2.28(3) and 3.47(3) Å] distances are very high. The "$AgSO_2$" geometry (bond lengths and angles) in **1** is comparable to that in $Ag(SO_2)[Al(OC(CF_3)_3)_4]$ [5] (S2.1.6/S2.1.7).



a) "$AgSO_2$" in **1**



b) "$AgSO_2$" in $Ag(SO_2)[Al(OC(CF_3)_3)_4]$

Figure S2.1.6: Comparison of "$AgSO_2$" in **1** (containing one of the three disordered SO_2 molecules) and in $Ag(SO_2)[Al(OC(CF_3)_3)_4]$

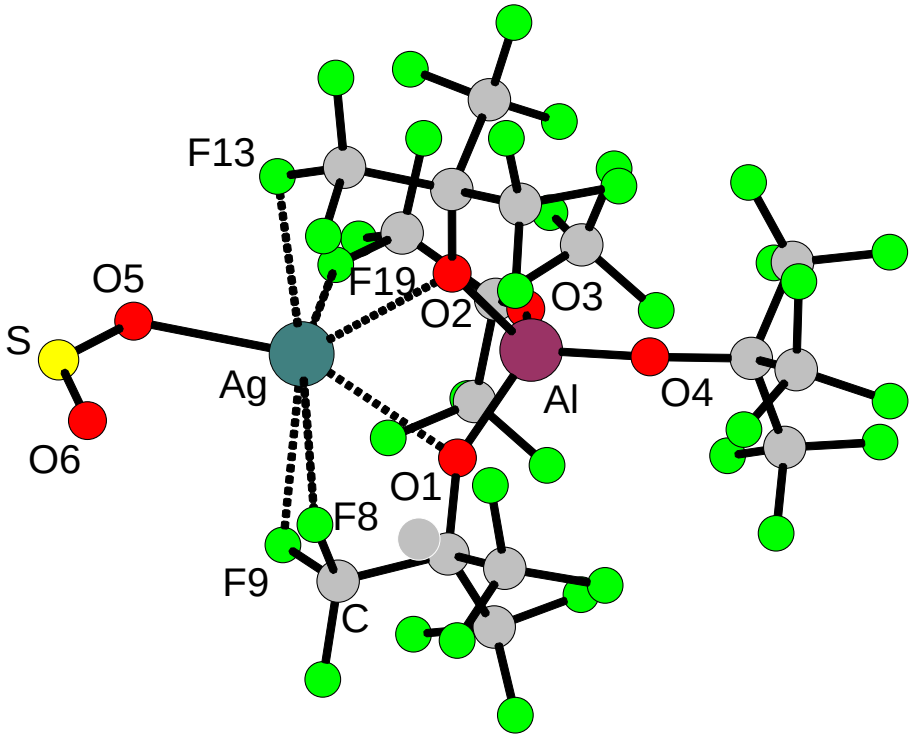


Figure S2.1.7: Crystal structure of $[Ag(OSO)][Al(OC(CF_3)_3)_4]$.

Each silver atom has three equivalent fluorine contacts (d(Ag-F) = 2.988(4) Å) which are shorter than the sum of their Van der Waals radii (3.20 Å)(S2.1.4). All other contacts are greater than 4.154 Å. This may be compared to similar Ag-F contacts in $[Ag(CH_2Cl_2)_2]_2[Ti(OTeF_5)_6]$ which lie between 3.028(7) and 3.034(7) Å. $[Ag(CH_2Br_2)_3][Sb(OTeF_5)_6]$ has only one Ag-F contact at d(Ag-F) = 3.196(7) Å.[6] Since $Ti(OTe_5)_6^{2-}$ is a (more basic) dianion and the Ag-F contacts in both species are longer than those observed in **1** this suggests the presence of a more electrophilic (electron deficient) Ag atom in $[(OSO)AgSe_6Ag(OSO)][Sb(OTeF_5)_6]_2$. However, if one compares the above given Ag-F contacts of about 2.99 to 3.20 Å to the shorter Ag-F interactions in $[Ag(PPh_3)_2][BF_4]$ (2.67 Å) and $[Ag(PPh_3)_2(CH_3CN)][BF_4]$ (2.65 Å),[7] the $[M(OTeF_5)_6]^{n-}$ (M= Sb, Ti, n = 1, 2) anions are seen to be very weakly coordinating. Ag-F contacts are provided by one fluorine atom from each of the three anions of one of the triangular faces of the octahedron surrounding the dication. The silver atoms are seven-coordinated (S2.1.8), common to more ionic Ag+ complexes.[8] A similar environment to the silver atom despite Ag-F contacts in **1** is found in $[Ag_4I_4(PPh_3)_4]$ containing a $(AgI)_4$ heterocubane core and terminal PPh_3 ligands, i.e. the Se atoms in (S2.1.8) are replaced by iodine and the oxygen atom (X) by phosphorus.[9]

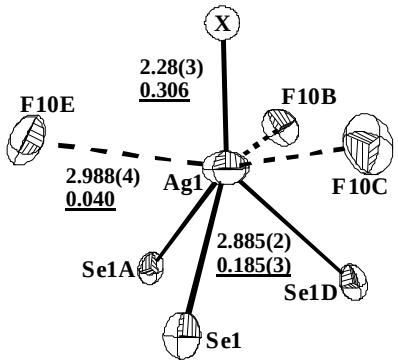


Figure S2.1.8: Coordinative environment of the Ag1 atom in **1**. X denotes the centre of the three disordered oxygen positions of the coordinated OSO. Bond length: Å, bond valence: v.u. The thermal ellipsoid are drawn at the 25% probability level.

The almost spherical $[Sb(OTeF_5)_6]^-$ anion consists of a central SbO_6 octahedron and six surrounding $OTeF_5$ octahedra (Fig. S2.1.9). Axial and equatorial Te-F bond lengths are indistinguishable within the

standard deviations and range from 1.77(2) to 1.839(8) Å. One of the two $OTeF_5$ groups in the asymmetric unit of **1** is rotationally disordered. Two orientations of the four equatorial fluorine atoms are occupied in a 60 : 40 ratio. Average Te-F [1.810(7-20) Å], Te-O [1.829(6)] and Sb-O [1.946(7) Å] distances and average Sb-O-Te bond angles of 142.1(4) ^{o} are in the range of other known $[Sb(OTeF_5)_6]^-$ anions.[10]

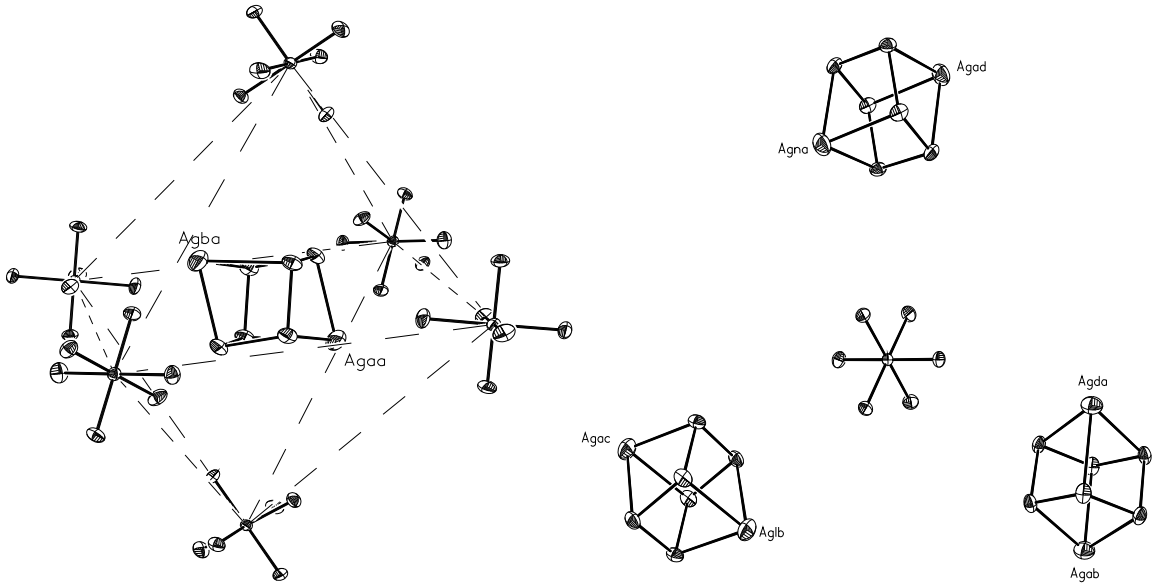


Figure S2.1.9: Ortep representations of the octahedral cation and trigonal anion environment in $[(OSO)AgSe_6Ag(OSO)][Sb(OTeF_5)_6]_2$ **1**. All fluorine, tellurium atoms and the SO_2 molecules are omitted for clarity. Thermal ellipsoids are drawn at the 25 % probability level.

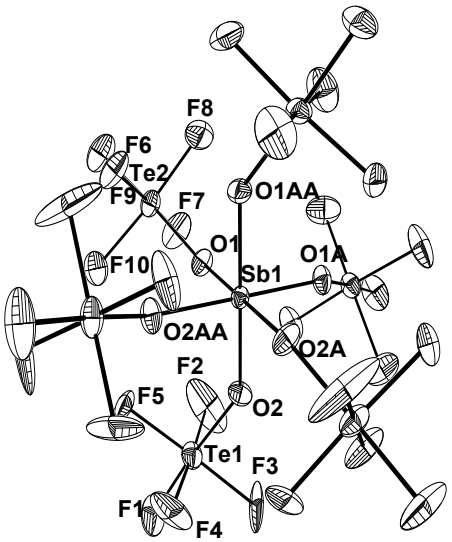


Figure S2.1.10: The $Sb(OTeF_5)_6^-$ anions in **1**. Thermal ellipsoids are drawn at the 25 % probability level.

Table S2.1.11: Structural parameters of the $Sb(OTeF_5)_6^-$ anions

Parameters	$[NR_4][Sb(OTeF_5)_6]$ R = Me	R = Et	**1**
$d(Te\text{-}F_{ax})_{av.}$	1.79(2)	1.76(2)	1.811(7)
Range			1.808(7)–1.814(7)
$d(Te\text{-}F_{eq})_{av.}$	1.74(2)	1.70(2)	1.809(7-20)
Range			1.77(2)–1.839(8)
$d(Te\text{-}O)_{av.}$	1.78(1)	1.74(1)	1.829(6)
$d(Sb\text{-}O)_{av.}$	1.91(1)	1.87(1)	1.946(7)
Sb-O-Te (av.)	150.9(8)	162.8(9)	142.1(4)
Range	148.4(8)-153.4(8)	160.7(9)–167(1)	141.0(4)-143.2(4)
R (R_w)	5.48 % (4.61 %)	7.10 % (5.99 %)	5.01 % (7.85 %)

S 2.2 Crystal structure of **2a**

2a: In contrast to **1** a single crystal X-ray structure determination of **2a** showed also the $[(OSO)AgSe6Ag(OSO)]^{2+}$ structural unit, but an additional SO_2 molecule is coordinated to each silver atom (Figure 1b in paper). The anion $[Al(OC(CF_3)_3)_4]^-$ forms double layers. Each double layer includes a slightly associated cation strand (S2.2.1).

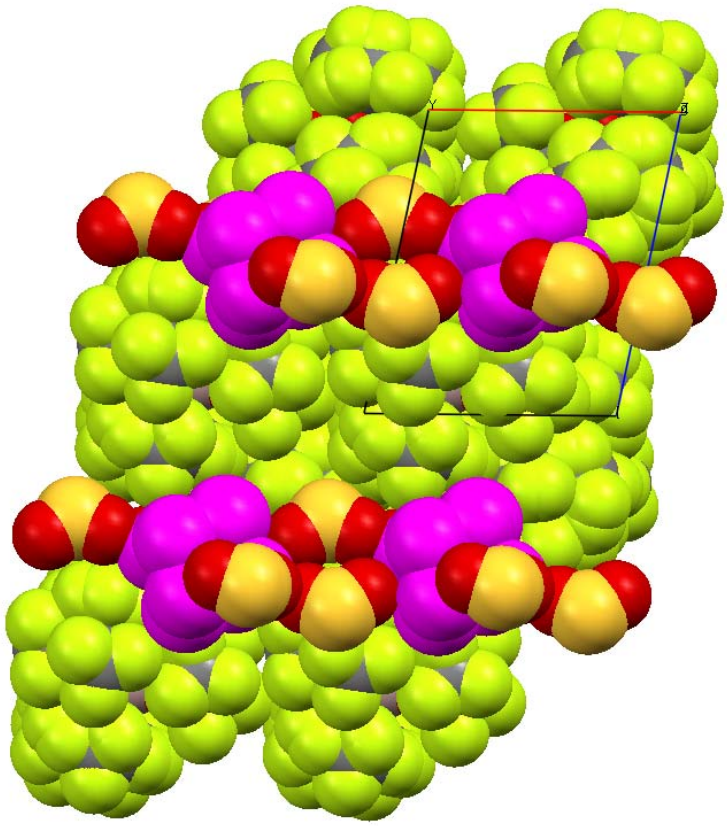


Figure S2.2.1: Space Filling representation of **2a** showing the anion double layer and the cation strand.

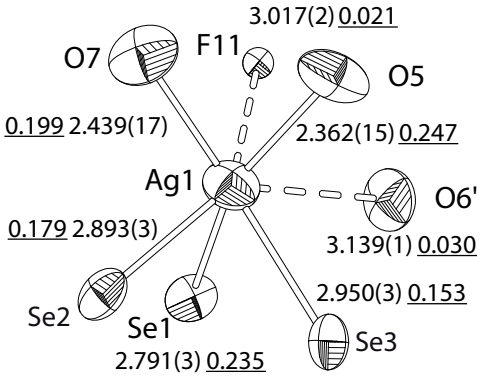


Figure S.2.2.2: Coordination Sphere of Ag1 in **2a**. O6' is a secondary contact to SO_2 coordinated to the next cation. Bond Valences v.u. are underlined. Distances in Å. The thermal ellipsoids are shown with 50% probability (F is isotropic).

The cation again contains a nearly D_{3d}-symmetric distorted $[Ag_2Se_6]$-cube and two types of SO_2-molecules coordinated to silver. One with a shorter Ag1-O3 distance of 2.362(15) Å; another one with a longer Ag1-O distance of 2.439(17) Å. The former has a secondary contact below the sum of van der

Waals radii to the silver atom of the next cation (d = 3.139 Å) and vice versa, resulting in a kind of double bridge (Figure S2.2.3).

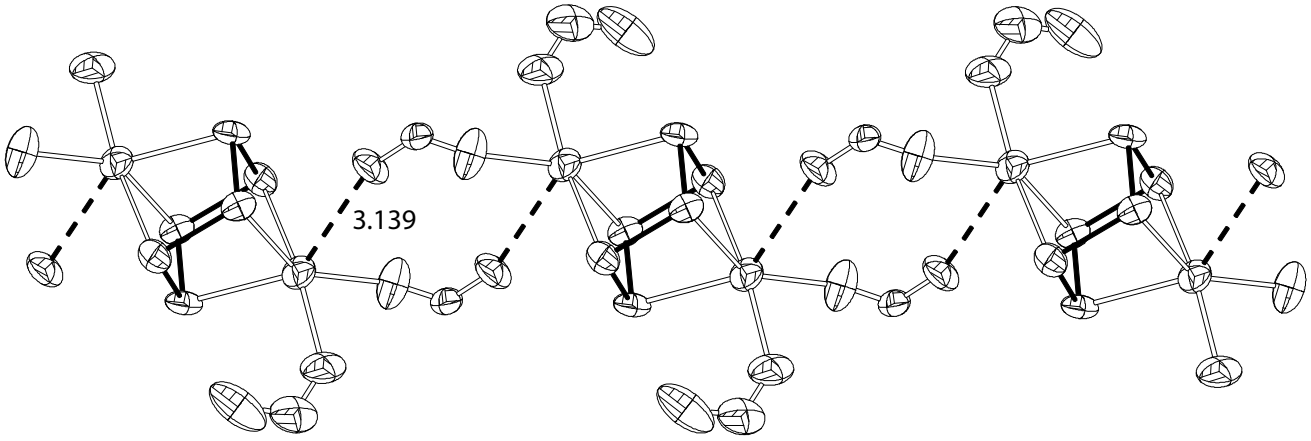


Figure S2.2.3: Section of the cation layer of **2** with Ag – O contacts (dashed lines/distance in Å). Thermal ellipsoids are shown with 50% probability.

Moreover five F-(O-S-O) (2xO/2xS/1xO) contacts within a limit of 3.20 Å are found (contacts to disordered F atoms in minority positions are not taken into account). The latter SO_2 points at the voids of the anion layer and thus prevents formation of directing Ag---F contacts and thus leads to the formation of completely disordered $C(CF_3)_3$ moieties in the proximity. On the one hand the $[Ag(OSO)_2]$-unit is comparable to **1** and $[Ag(OSO)][Al(OC(CF_3)_3)_4]$[5] with somewhat longer Ag1-O bond distances, on the other hand to $[Ag(OSO)_{2/2}][SbF_6]$[5]which features a true η_2-O,O' bridging, also found in the lithium salt $[Li_2(SO_2)_8][B_{12}Cl_{12}]$[11].

All S-O distances (d(SO) = 1.344(16), 1.402(14), 1.36(3), 1.406(19)) appear slightly shorter than in gaseous SO_2, likely due to libration and/or disorder. The (Ag-)OSO(-Ag) angle is greater (121.6°) and shorter (Ag-)OSO (116.3°) than in gaseous SO_2 (119.5°)[12].

The $[Ag_2Se_6]$-heterocubane itself also contains the Se_6-ring in chair conformation, the structural parameters of which are in very good agreement with Se_6 and **1** (Table 1, Figure 1 in the main text). There are three different Ag-Se distances (d(Ag1-Se1)= 2.791(3) Å; d(Ag1-Se2)=2.893(3) Å; d(Ag1-Se3)=2.950(3) Å) representing the deviation from ideal D_{3d}-symmetry. Compared to **1** (D_{3d}), over

$Se_6I_2^{2+}$ (C_{2h}) this is a symmetry reduction to point group C_i. This may be due to the asymmetry of different coordination sites to silver as well as packing effects.

Moreover there is a Ag-F-contact (below the sum of vdW radii of 3.014 Å which is in good agreement distances discussed in the previous section (Figure S2.2.2). Thus in addition to the Ag-O secondary contact Silver shows a seven-fold coordination, favoured in those compounds. This is analogous to **1** in which the silver atom bears three fluorine contacts. The valence sum[13] is 1.063 and close to one. This is again an example for the electron deficiency of Ag^+ saturated through OSO directly (1st sphere) and F/O indirectly (2nd sphere). Moreover several Se-F contacts (<3.2 Å) are found speaking of positive charge delocalization from silver to selenium. (S2.2.3)

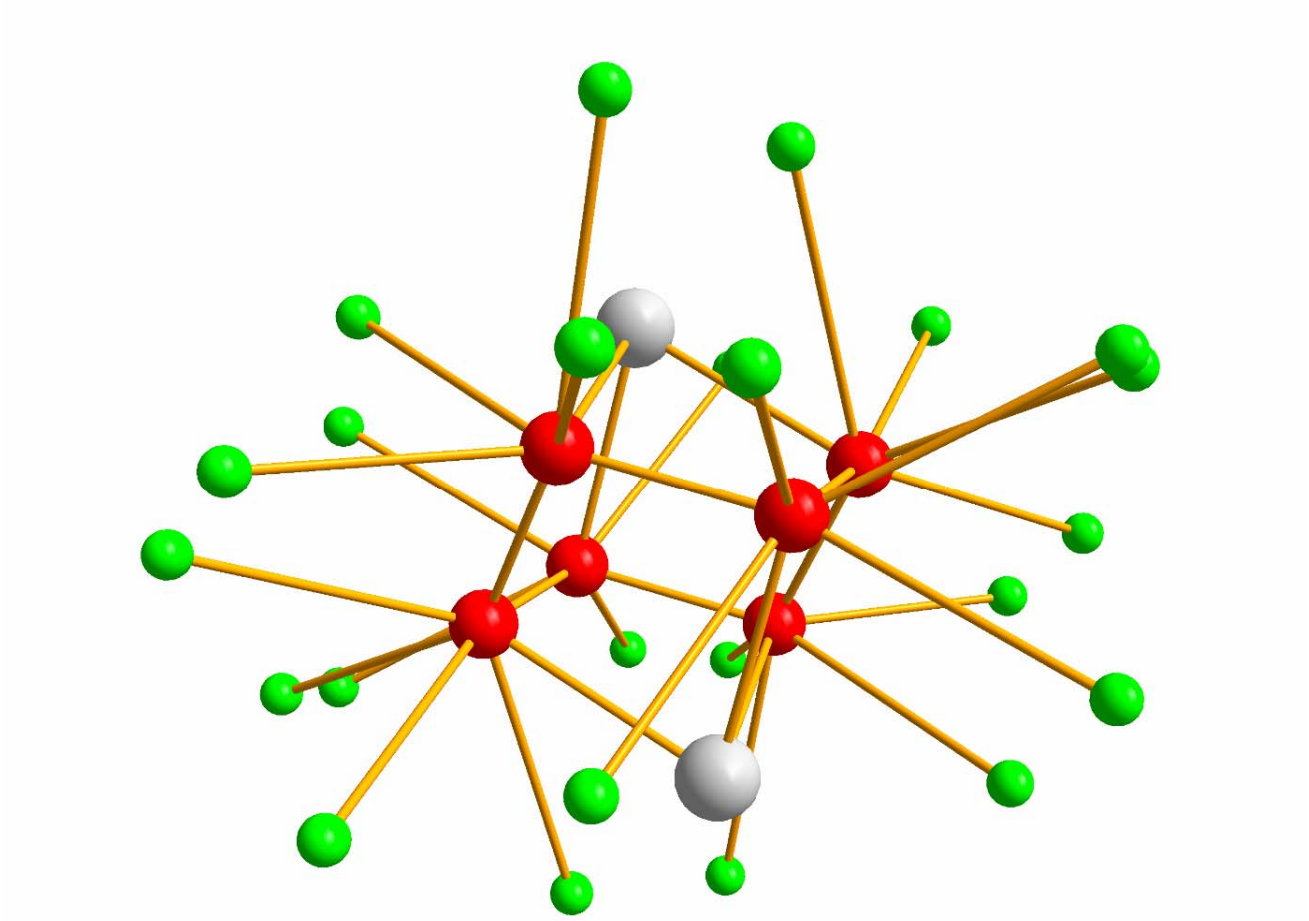


Figure S2.2.3: Se –F contacts below 3.2 Å in **2**.

The anion $[Al(OC(CF_3)_3)_4]^-$ is nearly spherical, contains a $[AlO_4]$-tetrahedron and shows rotational disorder of one CF_3 and of two $C(CF_3)_3$ groups (S2.2.4) which are typical for this kind of anion[14]. The disordered CF_3-group (occupation ratio 32 : 68) could not be refined anisotropically and therefore the contact to SO_2 leads to high standard deviations in the structural parameters. Moreover two perfluoro-*tert*-butoxy-groups are disordered, one with an occupation ratio of 55:45, another one with 35: 65. Major occupation sites could refined anisotropic, the minor sites were refined isotropic. Due to this disorder the data : parameter ratio reaches 7.9 / 1.[15]

The Al-O distances reach from 1.685(14) Å to 1.717(12) Å, typically for a highly disordered anion[16] and bearing uncommonly short Al-O bonds due to librational effects.

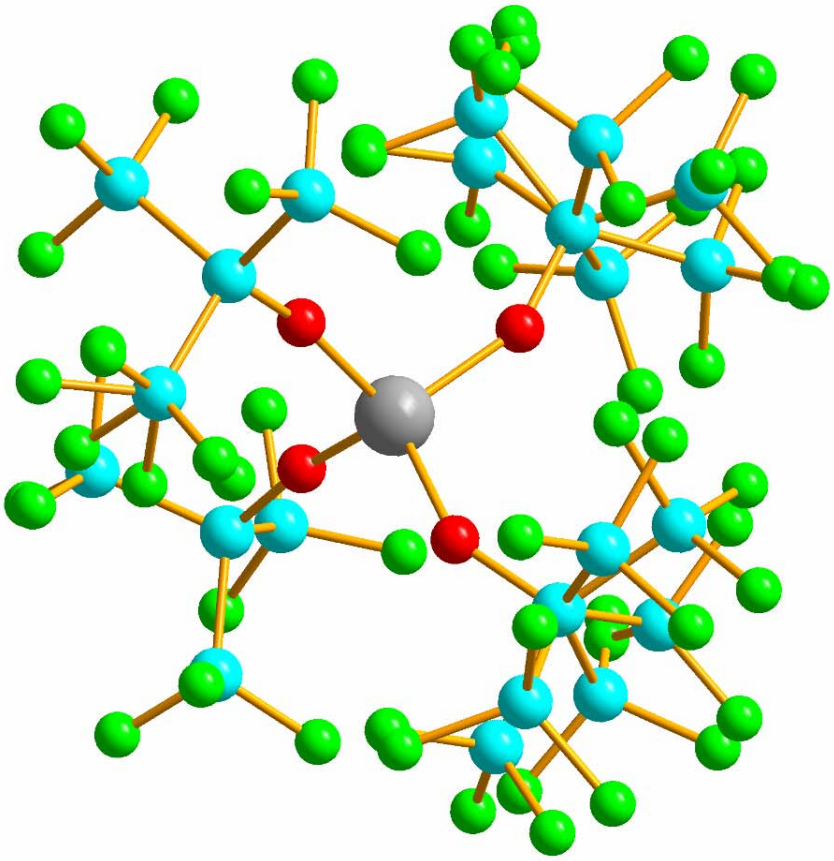
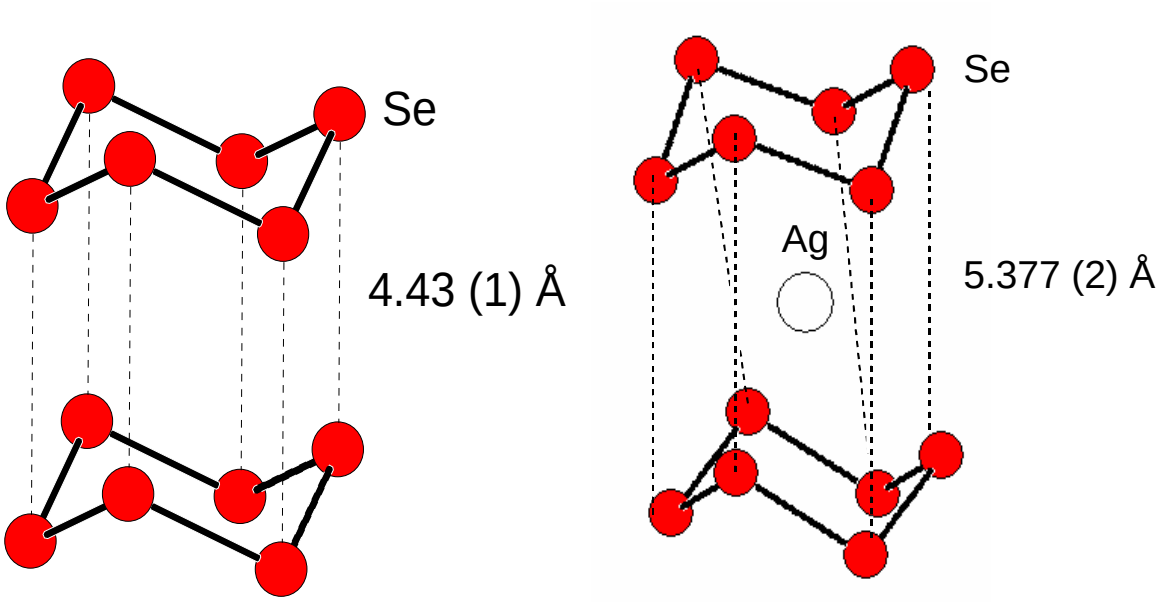


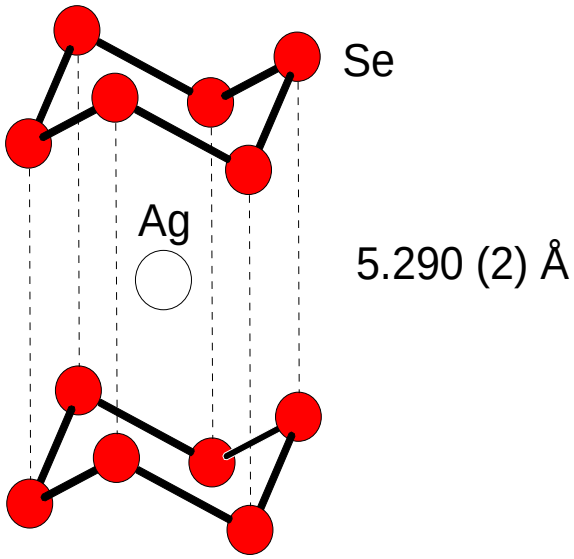
Figure S2.2.4: Representation of the disorder in the anion $[Al(OC(CF_3)_3)_4)]^-$ in **2a**.

S 2.3 Crystal structure of **3**

3: 3 is constructed from a polymeric $(AgSe_6^+)_n$ cation (see Figure 1b and 5a main text) and the honeycomb-like $[Ag_2(SbF_6)_3]^-$ anion (S2.3.5). The $(AgSe_6^+)_n$ cation can be viewed as containing a 1-dimensional polymeric chain of $(AgSe_6^+)_n$ cations containing a one dimensional stack of close packed Se_6 molecules with Ag^+ residing in the octahedral holes. This increases the distance between Se_6 molecules from 4.43(1) Å in Se_6 (solid)[17] to 5.377 (2) Å in **3**, and to 5.290 (2) Å in **4** (S2.3.1).



a) b)



c)

Figure S2.3.1: Distances between Se_6 rings in a) neutral Se_6 (s), b) **3**, and c) **4**. The distances were calculated as the average of the distances between corresponding Se atoms of adjacent Se_6 rings as indicated above.

A heterocubane like Ag1Se_6Ag1 portion of the stack is similar to the $Ag_2Se_6^{2+}$ core in **1** and **2**. Similar columns containing a metal ion and a ring of selenium, tellurium and arsenic are present in related species, e.g. $(RbSe_8^+)_n$ in $Rb_2[Pd(Se_4)_2]\cdot Se_8$ (S2.3.2)[18], $(CsTe_8^+)_n$ in Cs_4Te_{28},[19] $(MoAs_8^{2-})_n$ in $[K(2,2,2\text{-crypt})]_2[MoAs_8]\cdot NH_2(CH_2)_2NH_2$[20] and $[Rb(NbAs_8)^-]_n$ in $[Rb(2,2,2\text{- crypt})]_2[Rb(NbAs_8)]$.[21] It appears that the size and the coordination number of the group 15 and 16 rings are affected by the size of metal cation.

a) b)

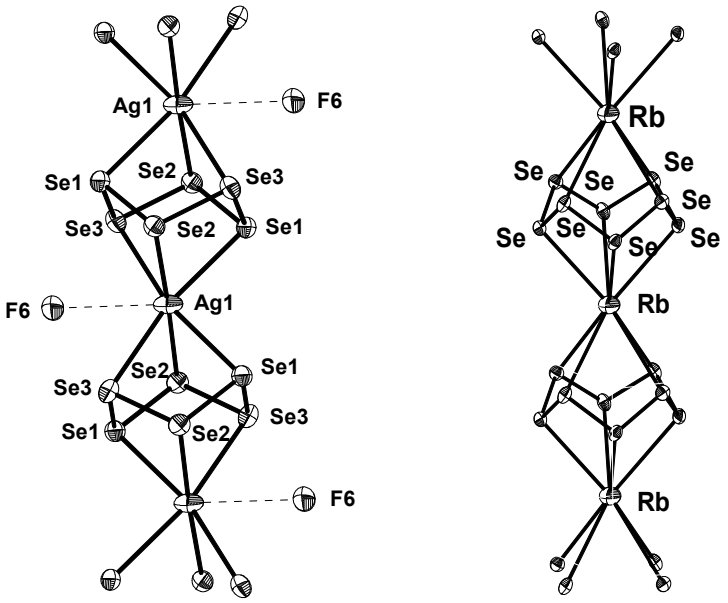
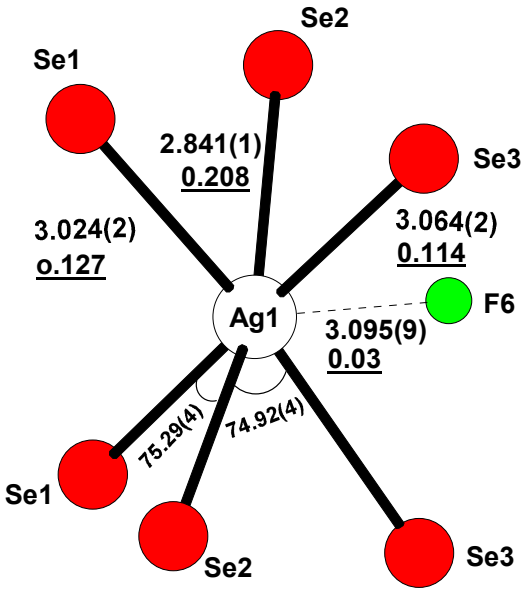
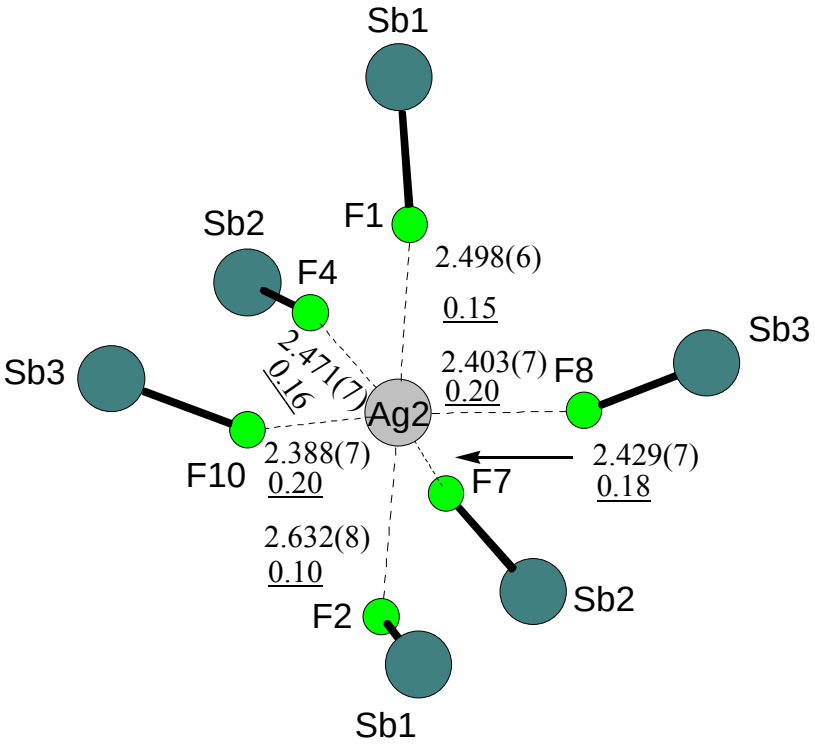


Figure S2.3.2: Structures of $(AgSe_6^+)_n$ in **3** and the $[Rb(Se_8)^+]$ chain cation in $Rb_2[Pd(Se_4)_2]\cdot Se_8$. The thermal ellipsoid are drawn at the 50% probability level.

The silver atom (Ag1) in the "Se_6Ag" chain has only one fluorine contact (d(Ag1-F6) = 3.095(9) Å, 0.03 v.u.; Σ van der Waals radii of Se and Ag^+ is 3.20 Å) (see Figure 5a and S2.3.3) in the second coordination sphere of Ag1.



a)



b)

Figure S2.3.3: Coordination spheres of Ag1 and Ag2 in **3**

Although the contact is weak, it directs the Ag^+ ion away from a straight line down the stack axis and leads to unequal Ag-Se bond lengths and SeAgSe angles (Figure 1b and S2.3.3). Each selenium atom has two contacts to the fluorine atoms (2.912(7) – 3.218(8) Å), which are below the sum of their van der Waals radii (3.40 Å) (S2.3.4). These Ag1-F and Se-F contacts are comparable to those in **1** and **2**.

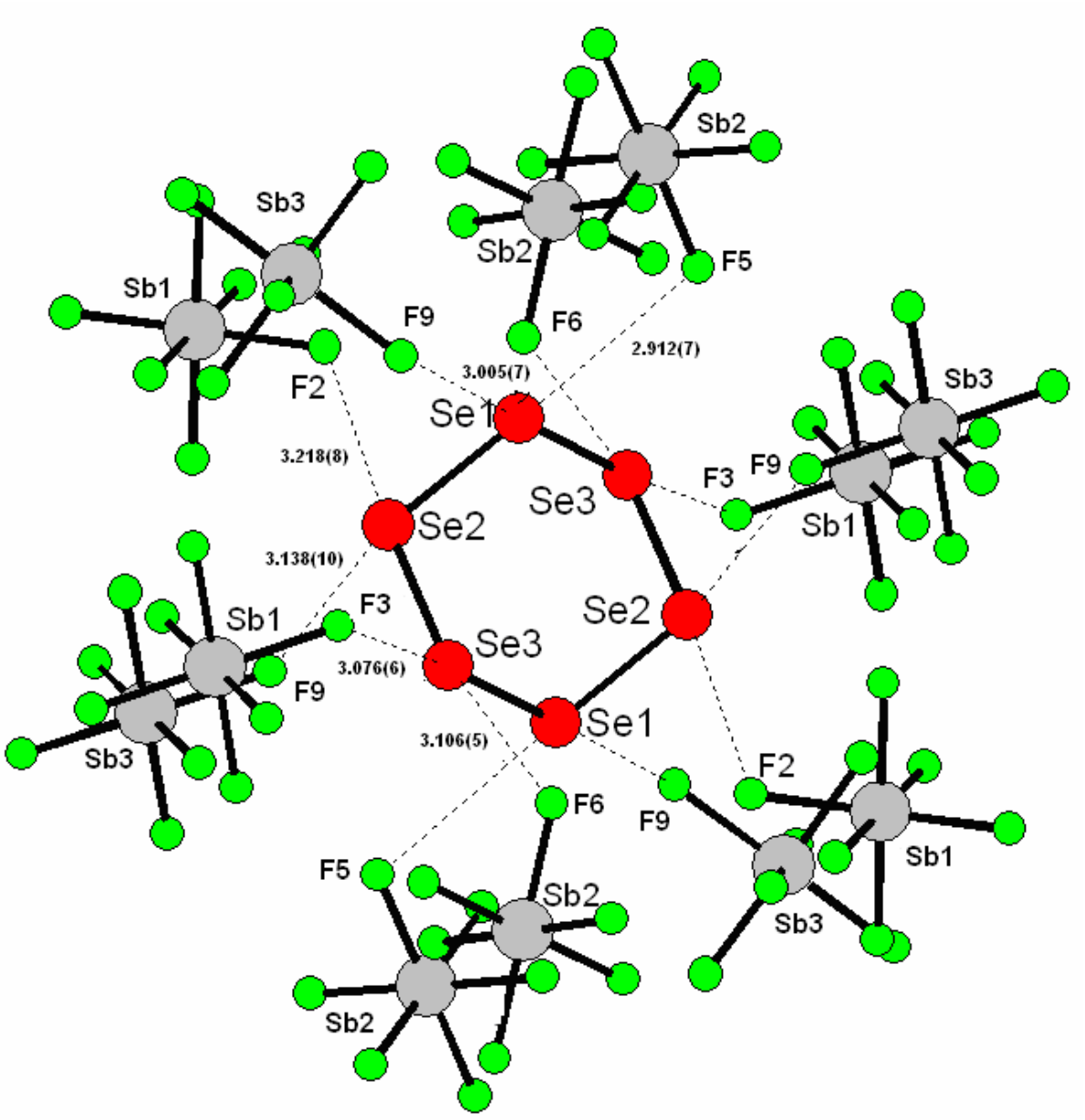
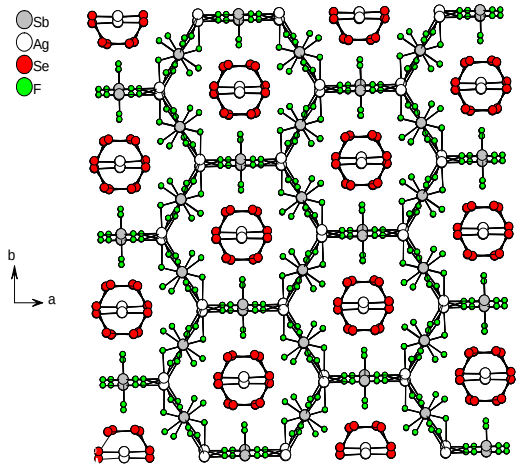
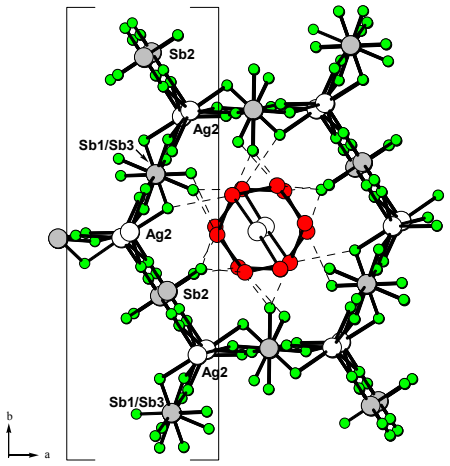


Figure S2.3.4: The anion-Se_6 contacts in **3**

The anion is constructed from two silver cations and three SbF_6^- anions per $[AgSe_6]^+$ link of the polymeric cation chain. The hexagonal channels, in which the cationic chains reside, are formed by the interaction of silver cations with fluorine atoms from each SbF_6^- anions (Figure S2.3.5). Six silver atoms reside at each corner of the hexagonal cavity and contact six bridging SbF_6^- units (Figure S2.3.5 b) The surface of the channels along the a-axis can be viewed as an eight-membered ring (2 Sb, 4F and 2Ag) crossed net (Figure 2.3.5 c).



a)



b)

c)

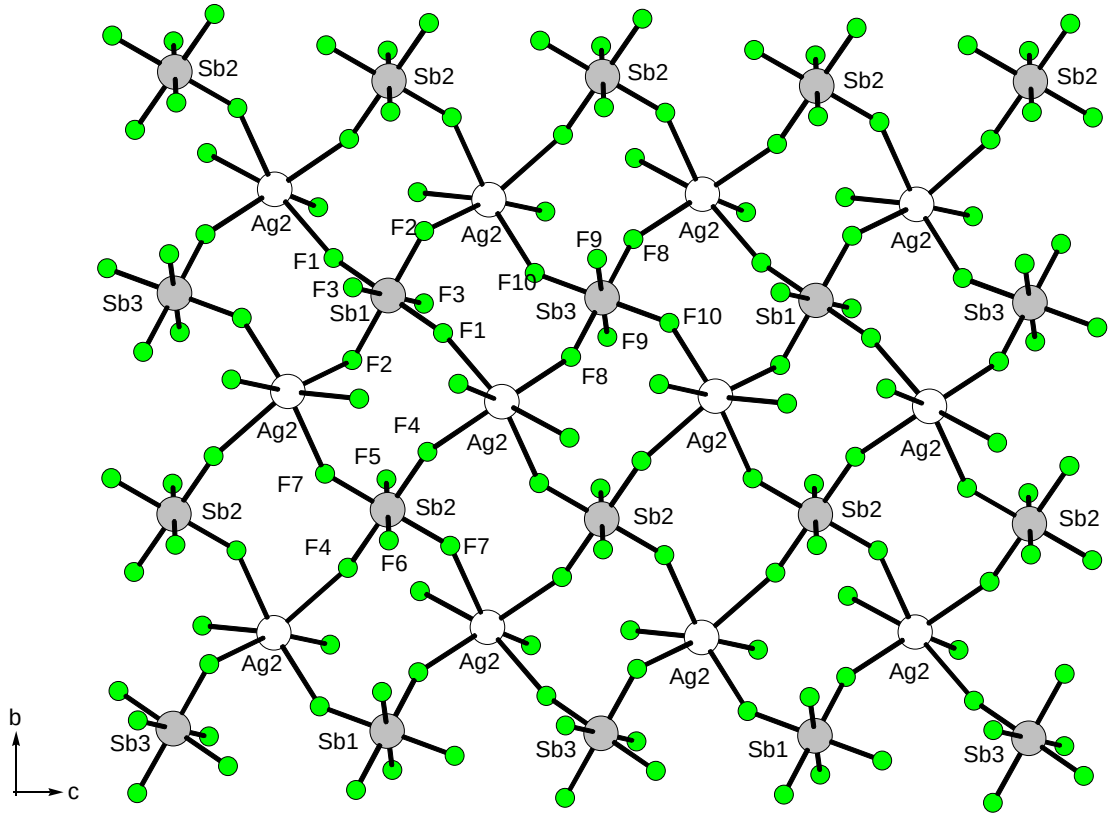
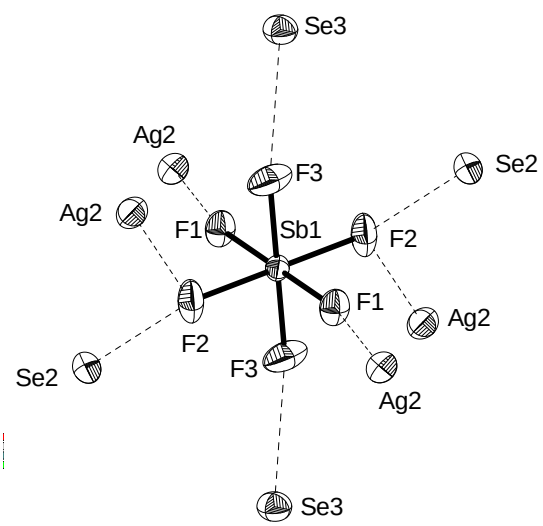
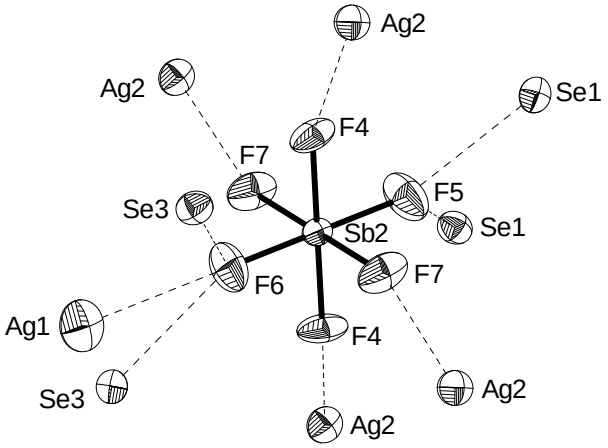


Figure 2.1.5: a) view of **3** down the c-axis; b) an expansion of a portion of 3 down the c-axis; c) a side-view down the a-axis of the highlighted part in the bracket of Figure b.

Three types of SbF_6^- units are observed within the complex anion, differing in the orientation towards their neighbouring silver atoms and towards the $[AgSe_6]^+$ chain. Each individual SbF_6^- unit is structurally unremarkable (Sb-F in range 1.859(6)-1.884(6) Å, F-Sb-F angles 90 ± 0.7 or 180 ± 0.2 °) (S2.3.6).

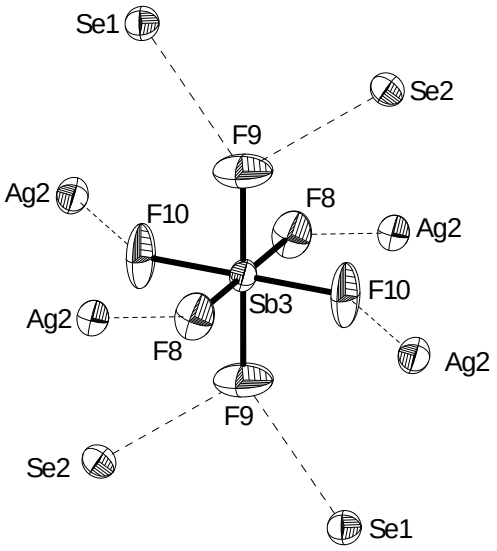


d(Sb1-F1) = 1.884(6), s = 0.80
d(Sb1-F2) = 1.876(7), s = 0.81
d(Sb1-F3) = 1.859(6), s = 0.85
Σs(Sb-F) = 4.92 v.u.



d(Sb2 - F4) = 1.869(6), s = 0.83
d(Sb2 - F5) = 1.864(10), s = 0.83
d(Sb2 - F6) = 1.868(10), s = 0.83
d(Sb2 - F7) = 1.866(7), s = 0.83

Σs(Sb2 - F) = 4.98



d(Sb3 - F8) = 1.883(7), s = 0.80
d(Sb3 - F9) = 1.866(7), s = 0.84
d(Sb3 - F10) = 1.871(7), s = 0.82

Σs(Sb - F) = 4.92 v.u.

Figure S2.3.6: Coordination spheres of $Sb1F_6^-$, $Sb2F_6^-$ and $Sb3F_6^-$ in **3**. Thermal ellipsoids are drawn at the 50 % probability level.

The Sb-F distances are essentially independent of whether the fluorine atoms are weakly linked to Ag^+ or the Se_6 ring of $(AgSe_6^+)_n$ implying the selenium atom in Se_6 are also positively charged. Sb1 and Sb3 are superimposed along the c-axis while the Sb2 atoms are alternatively displaced either side due to

the Sb2-F(6)---Ag1 interaction that leads to the distortion of the $(AgSe_6^+)_n$ stack (Figure 2.3.2 and S2.3.9).

Neutral chalcogenide rings stabilized in a host structure is relatively rare. There are even fewer metal chalcogenide complex directed 2D and 3D host structures. Several examples are reported as encapsulated in 2D host structures, such as $(Cs(S_8)^+)_n$ in $Cs_2Sn_3S_7{\cdot}0.5S_8$,[22] $[Cs(Te_8)^+]_n$ in Cs_3Te_{22}, and $[Rb(Se_8)^+]_n$ in $Rb_2[Pd(Se_4)_2]{\cdot}Se_8$ (Figure S2.3.7 a). Columns of $[Cs(Te_8)^+]_n$ in Cs_4Te_{28} are inserted into an anionic 3D telluride $[Te_{20}^{4-}]$ framework. Few examples[23-26] of host framework based on simple inorganic salts are known, all of which are constructed from $AgNO_3$ or from its components e.g. $Ag(NO_3)_3^{2-}$. A striking example is $C_{60}\{Ag(NO_3)\}_5$ in which the zeolithe-like $[(AgNO_3)_5]$ network hosts the fullerene guest. The polymeric $(Se_6Ag^+)_n$ promoted honeycomb-like net,[27-29] formed by $[Ag_2(SbF_6)_3^-]_n$ in **3** is comparable to that of $\{[Ag(NO_3)_3]^{2-}\}_n$ in $[Ag_5L_3(NO_3)_3][Ag(NO_3)_3]{\cdot}3CHCl_3$ (L = bipyridine-Schiff-base ligand) (Figure S2.3.7 b).

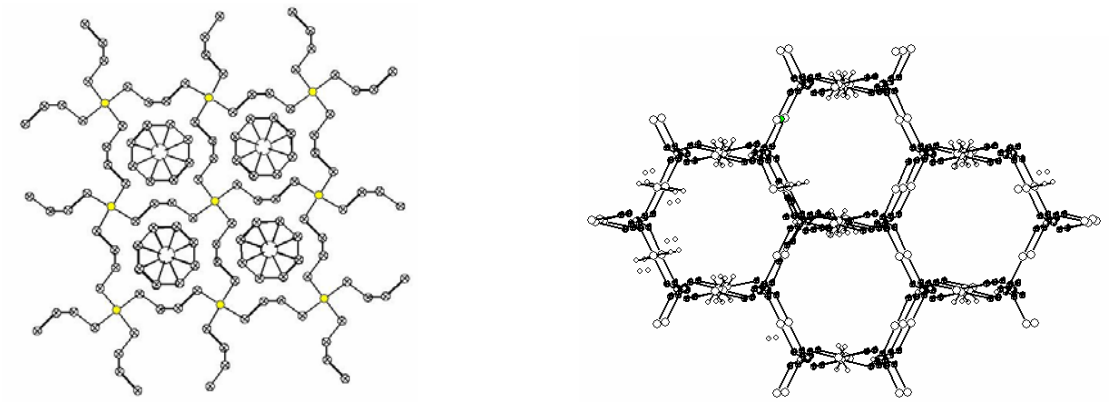


Figure S2.3.7: a) A view of $Rb_2[Pd(Se_4)_2]{\cdot}Se_8$; b) A view of the $[Ag(NO_3)^{2-}]_n$ framework in $[Ag_5L_3(NO_3)_3][Ag(NO_3)_3]{\cdot}3CHCl_3$ (L = bipyridine-Schiff-base ligand).

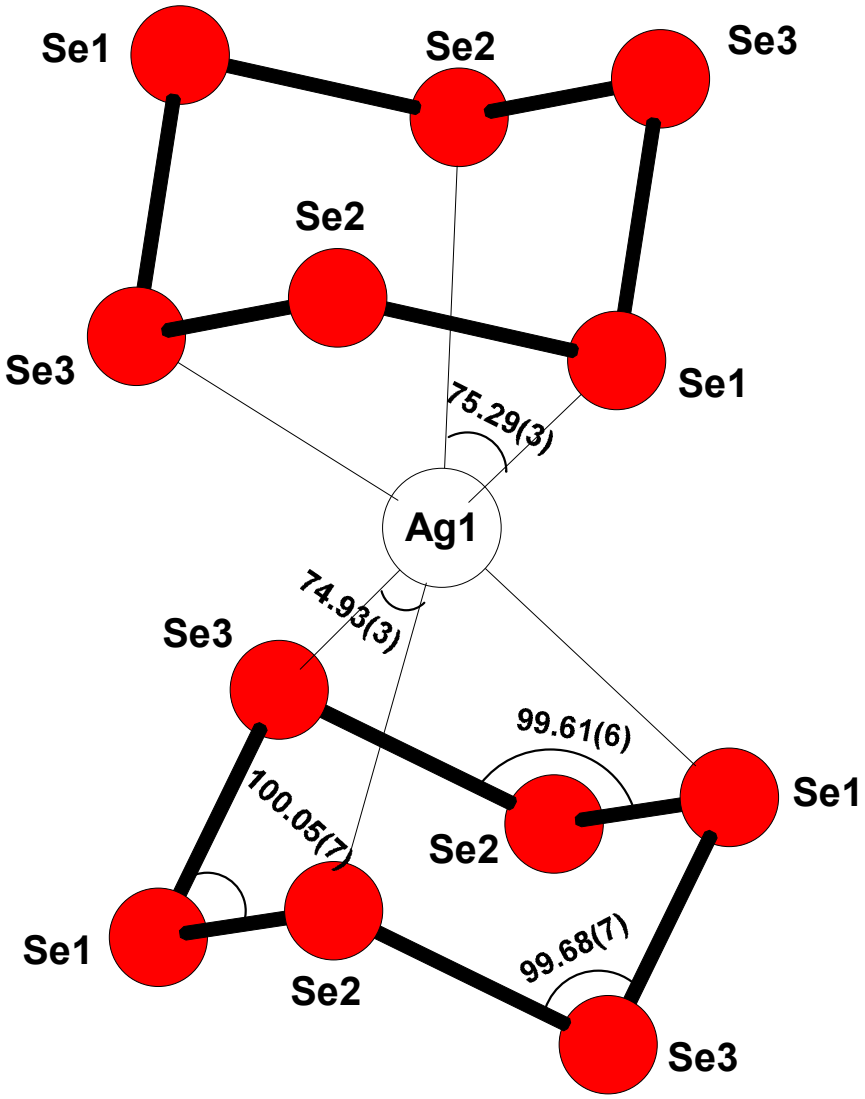


Figure S2.3.8: Bond angles in **3**

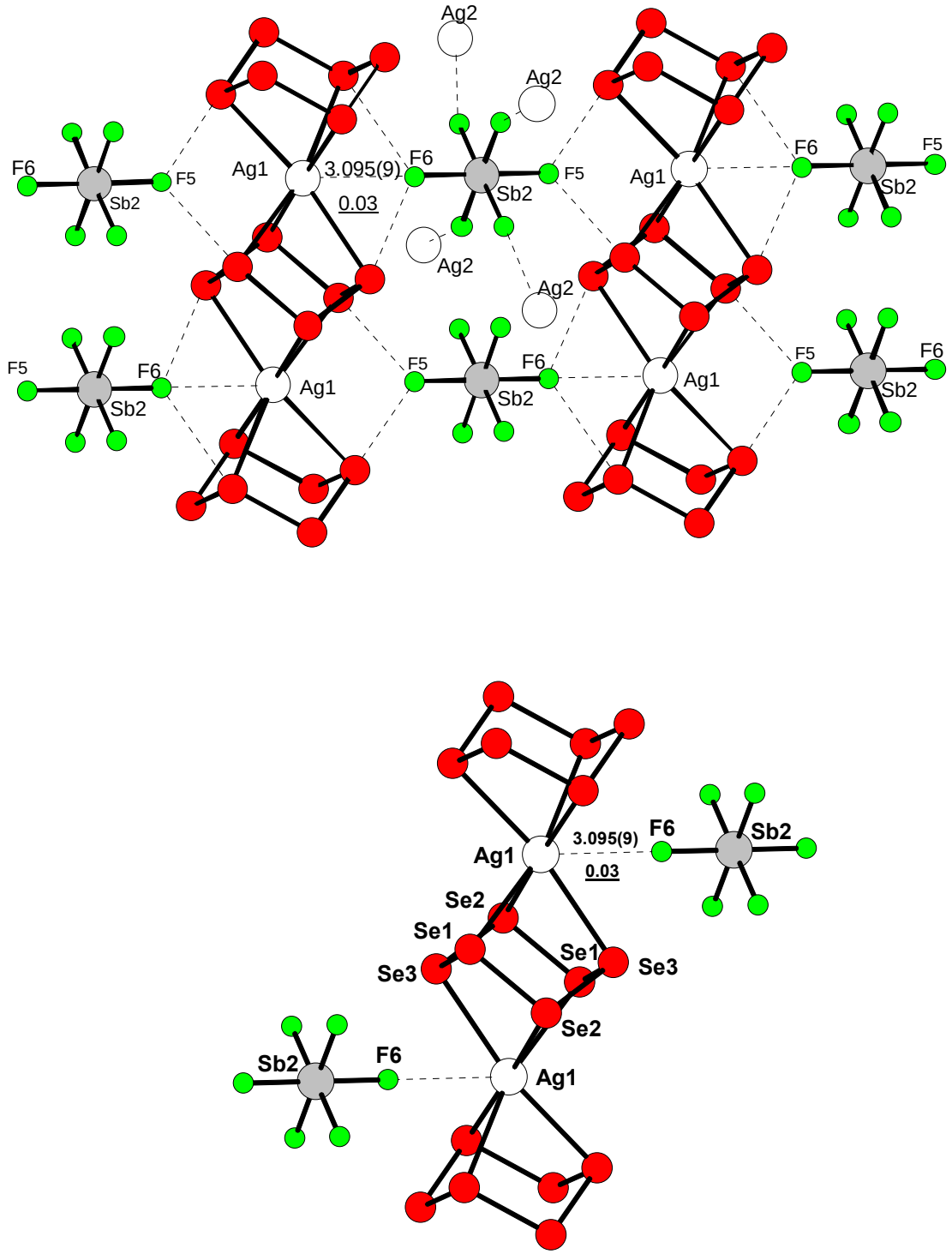


Figure S2.3.9: A detailed and simplified view of F6 (from Sb3)-Ag1 interactions in **3**

S 2.4 Crystal structure of **4**

4: The $[(AgSe_6Ag)^{2+}]_n$ cation in **4** consists of an infinite two-dimensional cation containing polymeric chains of $[Ag1Se_6^{+}]_n$ cross-linked by silver (Ag2) cations (Figure 1d in main text and S2.4.1).

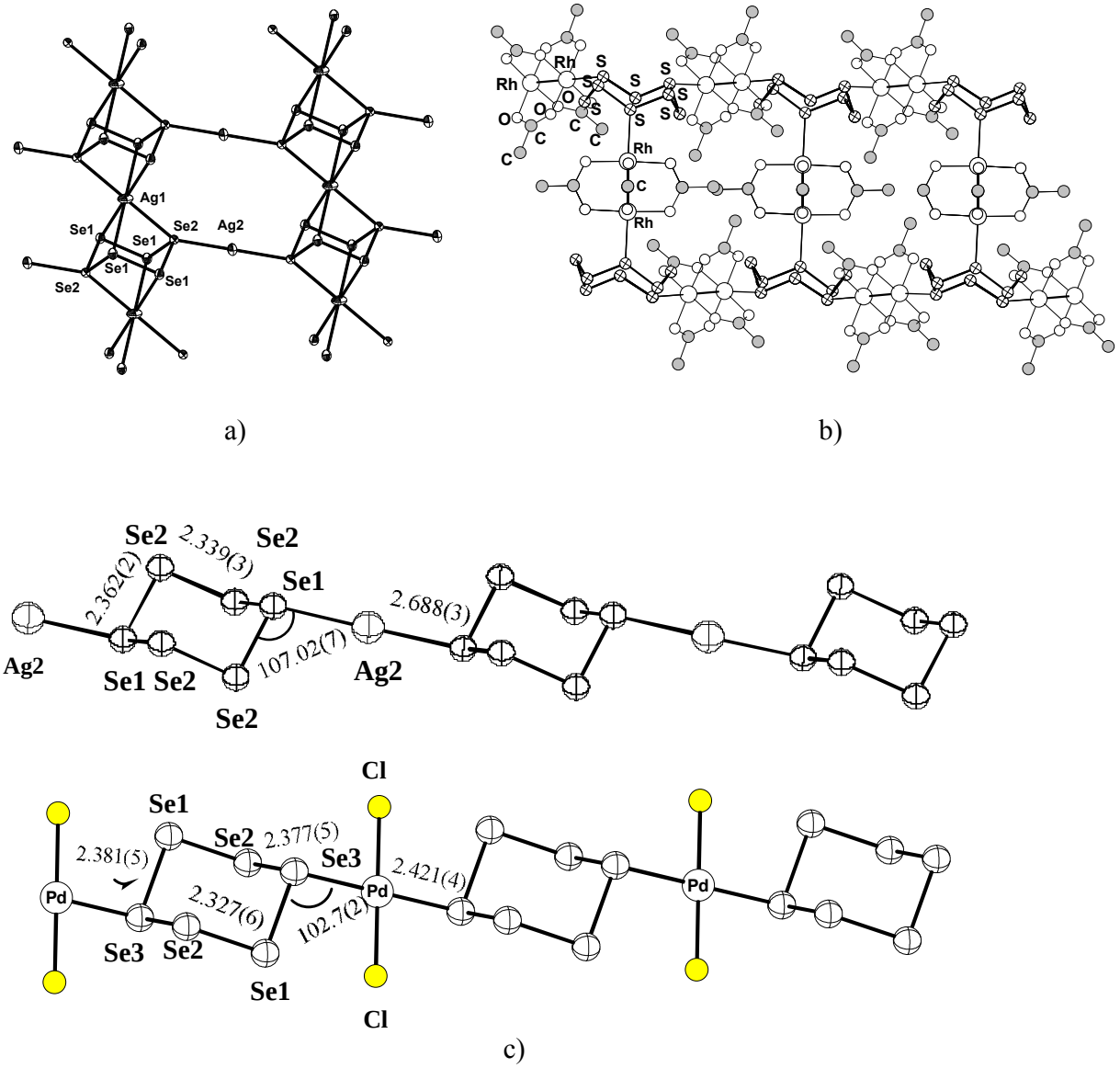


Figure S2.4.1: a) Structure of the $[(AgSe_6Ag)^{2+}]_n$ cation in **4**; The thermal ellipsoids are drawn at the 50% probability level; b) Structure of $[Rh_2(O_2CCF_3)_4]_3(S_8)_2$; c) Comparison of the "$(Ag2Se_6^{+})_n$" fragment in $[(AgSe_6Ag)^{2+}]_n$ and the $PdCl_2Se_6$ geometries in the solid state.

The $[Ag1Se_6^{+}]_n$ stacks can be described similarly as for the related stacks in **3**. Adjacent $[Ag1Se_6^{+}]_n$ stacks are linked by shorter, linear Se_6-Ag2-Se_6 bonds (Ag2-Se1 2.688(2) Å; Se1-Ag2-Se1 180.00(4)º). Alternatively, the $[(AgSe_6Ag)^{2+}]_n$ cation in **4** can be considered as built from polymeric $[Ag_2Se_6^{+}]_n$

chains cross-linked by silver (Ag1) cations. The $[Ag_2Se_6^+]_n$ chains are similar to those of $PdCl_2Se_6$ in which Se_6 is side-on coordinated to Pd (Figure S2.4.1 c).[30] Related cyclic S_8, Se_6, and Se_7 molecules usually coordinate side-on (as S_8 to Ag in AgS_8^+, Se_6 in **1** and **2**) or end-on (as Se_6 to Pd in $PdCl_2Se_6$, Se_7 to Re in $Re_2I_2(CO)_6Se_7$[31, 32]). The infinite 2D architecture in $[(AgSe_6Ag)^{2+}]_n$ contains both side-on and end-on coordination modes. As far as we are aware, such a 2D structure constructed from simple components has not been previously observed. However a related pseudo 2D ribbon-type structure in $[Rh_2(O_2CCF_3)_4)_3(S_8)_2]_n$ has been reported by F. A. Cotton and his coworkers,[33] in which two infinite chains of $[Rh_2(O_2CCF_3)_4(S_8)]_n$ are further connected by additional dirhodium tetra(trifluoroacetate) molecules lying between each pair of facing S_8 rings (Figure S2.4.1 b).

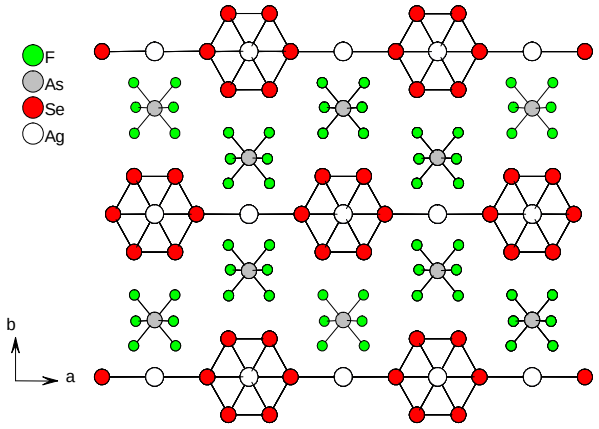
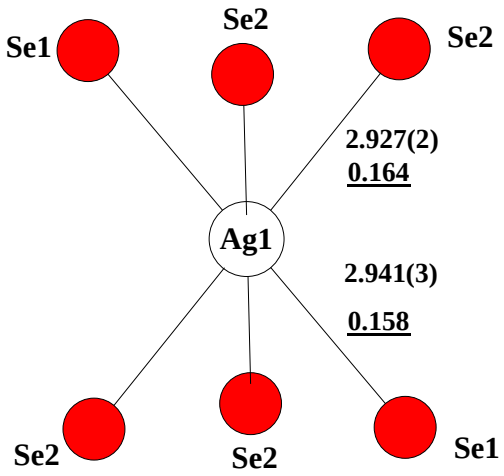
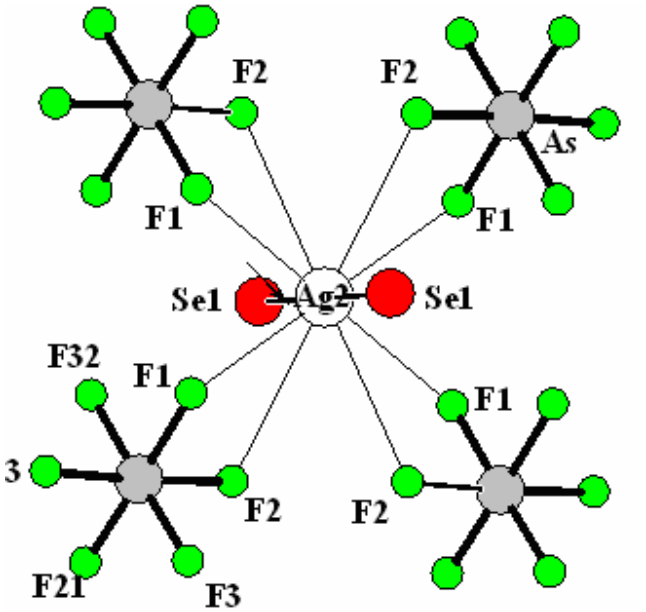


Figure S2.4.2: A portion of **4** projected down the c-axis.

The overall structure of **4** consists of sheets of $(AgSe_6Ag^{2+})_n$ in the ac plane and separated by AsF_6^- anions, linked by fluorine-cation contacts (Figure S2.4.2). Each $AgSe_6$ fragment is surrounded by six AsF_6^- anions. There are no Ag-F contacts to the $(Ag1Se_6^+)_n$ chains in **4**. In contrast, the bridged Ag2 in **4** is involved in multiple fluorine contacts, two from each of the four adjacent anions (Ag2-F1 2.689(6) (x 4), Ag2-F2 3.053(6) (x 4) Å). Each selenium atom in **4** has four (Se1) or five (Se2) contacts to fluorine (S2.4.5) with Se-F distances similar to those in **3**. The bond distances in the AsF_6^- (C_2) anion in **4** can be found in figure S2.4.7.



Σ(Ag1-Se) =0.966



d(Ag2 - F1) = 2.689(6), s = 0.09
d(Ag2 - F2) = 3.053(6), s = 0.034
d(Ag1 - Se2) = 2.688(2), s =0.31
Σs(Ag2 - F/Se) = 1.116

Figure S2.4.3: Coordination spheres of Ag1 and Ag2 in **4**

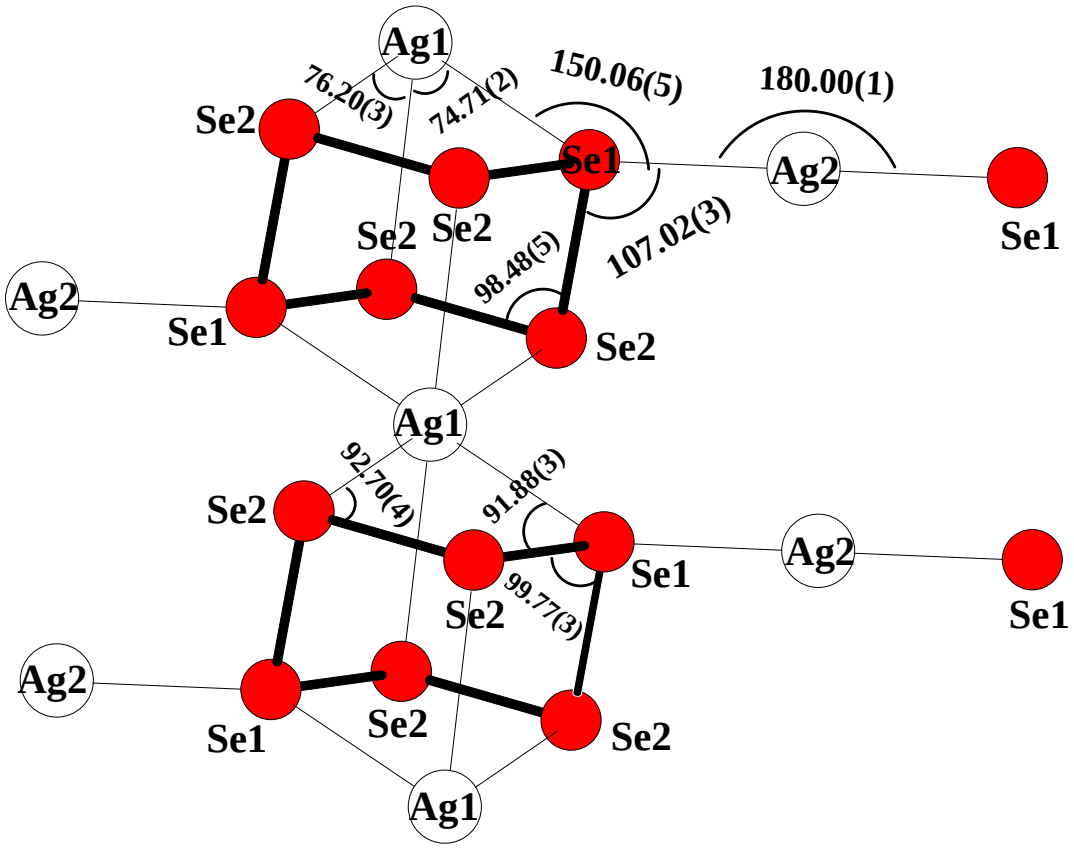


Figure S2.4.4: Bond angles in **4**

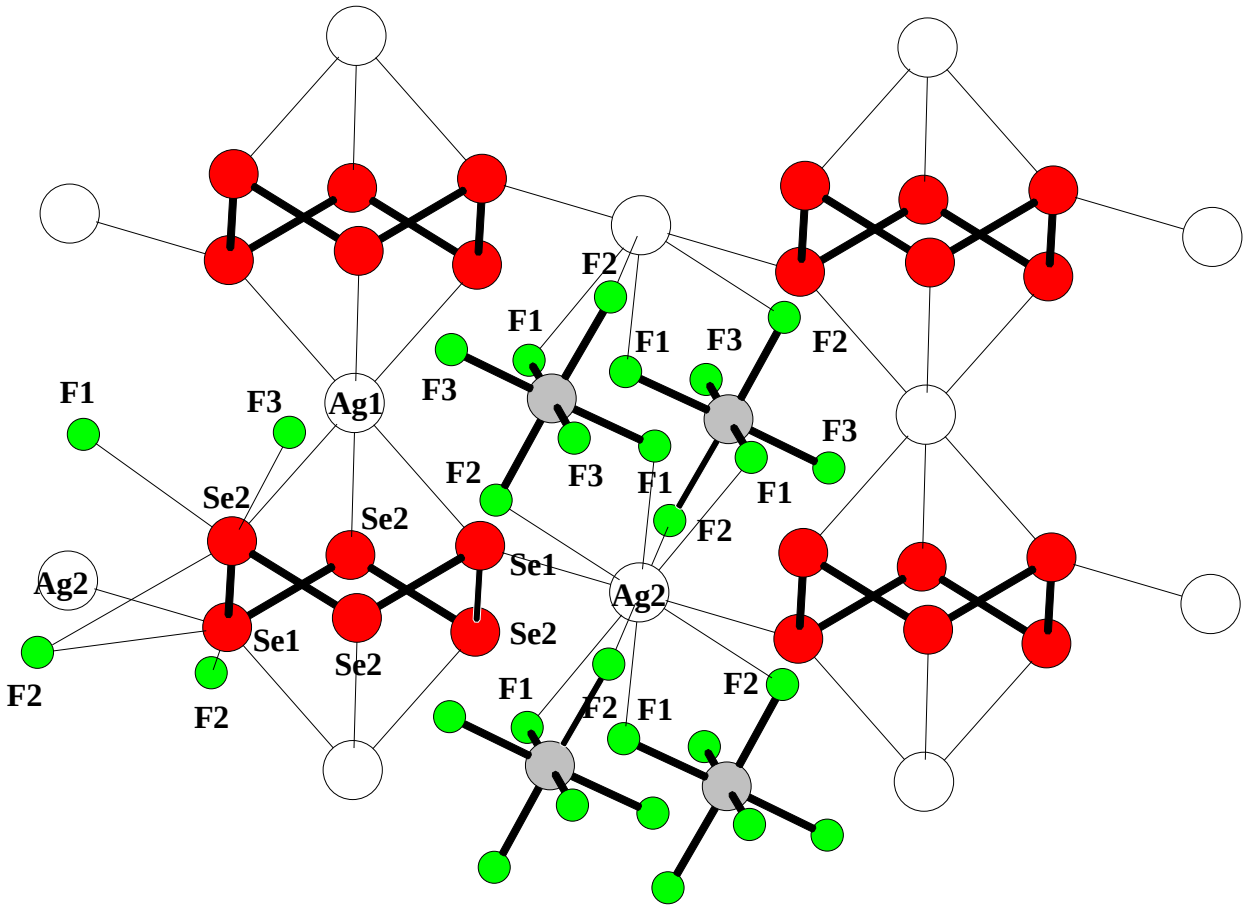
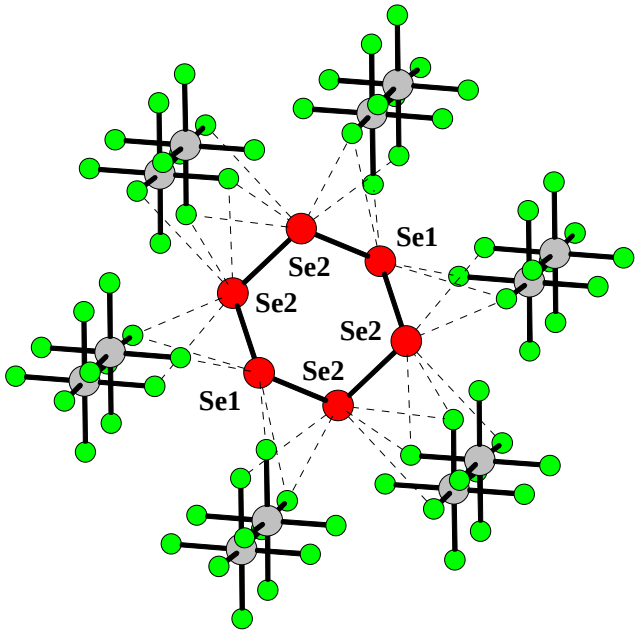
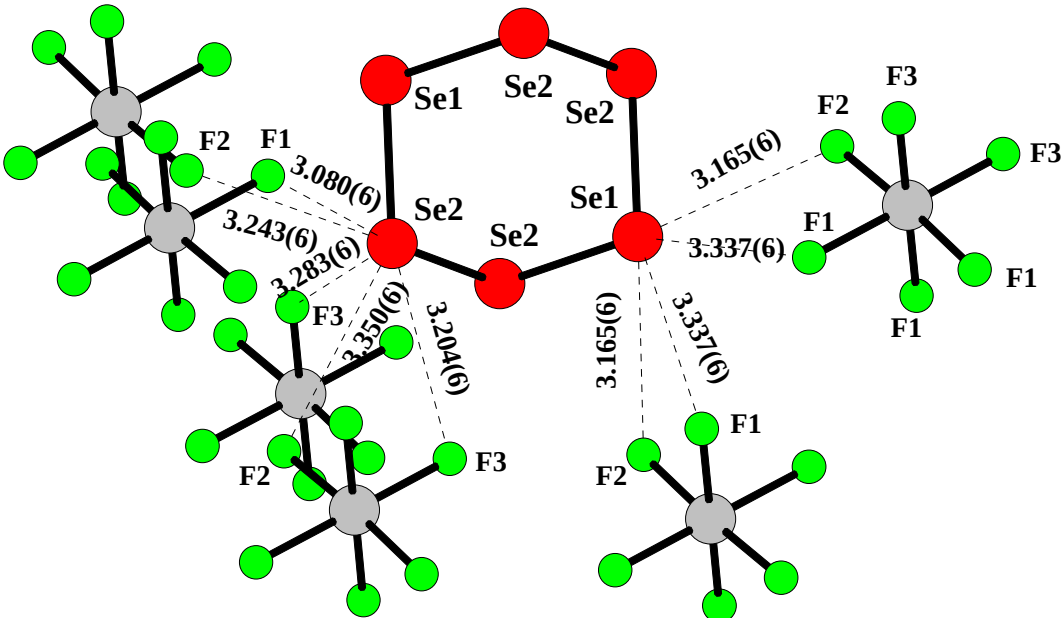


Figure S2.4.5: Cation-anion interactions in **4**



a)



b)

Figure S2.4.6: a) Se_6-anion interactions in **4**; b) Se1-F and Se2-F bond distances

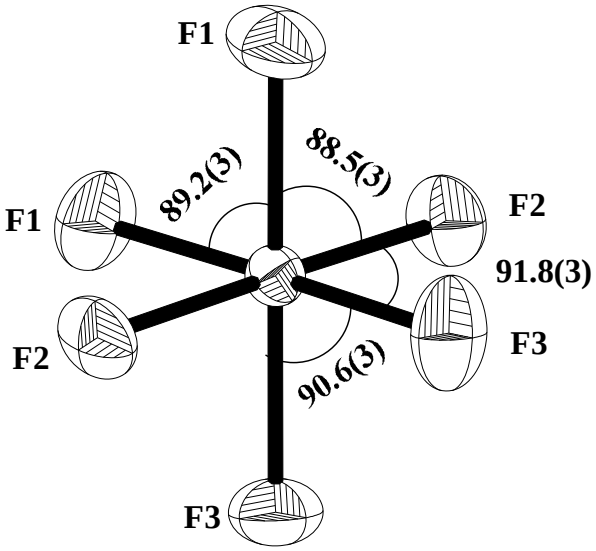


Figure S2.4.7: Coordination sphere of As in **4**. As-F1 = 1.721 (5), As-F2 = 1.712(5), As-F3 = 1.688 (6) Å. The thermal ellipsoids were drawn at the 50% probability level.

Table S2.5: Comparison of the structural parameters of Se_6 rings in several structures including 1-4 and A-E.

	Se6 (s)[a]	1	2	3	4	$Cu_2Br_2Se_6$[b]	$PdCl_2Se_6$[c]	$(Se_6I)_n\ n(SbF_6)$[d]	$Se_6I_2[AsF_6]_2 \cdot 2\ SO_2$[d]	$Se_6(Ph)_2(AsF_6)_2 \cdot SO_2$[e]	$Rb_3AsSe_4 \cdot 2\ Se_6$[f]		
Se-Se(Å)	2.356 (3)	2.346 (2)	2.339(3) (x2)	2.346 (2) (x 4)	2.339 (3) (x 2)	2.354(4) (x 4)	2.327 (6) (x 2)	2.295 (4) (x 2)	2.227 (2) (x 2)	2.263 (4) (x 2)	2.367 (2)		
(in the Se6 ring)			2.368(3) (x2)	2.345 (2) (x 2)	2.362 (2) (x 4)	2.389 (3) (x 2)	2.377 (5) (x 2)	2.362 (3) (x 2)	2.468 (2) (x 2)	2.383 (3) (x 2)			
			2.353(3) (x2)				2.381 (5) (x 2)	2.365 (4) (x 2)	2.482 (2) (x 2)	2.449 (4) (x 2)			
Se-Se(ave., Å)	2.356 (3)	2.346 (2)	2.353(3)	2.346 (2)	2.354 (3)	2.366 (4)	2.362 (5)	2.341 (4)	2.392 (2)	2.365 (4)	2.367 (2)		
Se-Se-Se(o)	101.1 (1)	100.91 (7)	100.16(10) (x2)	99.61 (7) (x 2)	98.48 (7) (x 4)	99.06 (15) (x 2)	97.7 (1) (x 2)	103.3(1) (x 2)	95.72(7) (x 2)	99.61 (1) (x 2)	102.93 (6)		
			100.55(10) (x2)	99.68 (6) (x 2)	99.76 (9) (x 2)	100.85 (13) (x 4)	98.8 (2) (x 2)	103.7 (1) (x 2)	103.48(7) (x 4)	100.1 (1) (x 2)			
			99.75(10) (x2)	100.05 (6) (x2)			107.7 (1) (x 2)	104.3 (1) (x 2)		102.4 (1) (x 2)			
Se-Se-Se(ave., o)	101.1 (1)	100.91 (7)	100.15(10)	99.78(2)	98.91 (5)	100.25 (13)	101.4 (1)	103.8 (1)	100.89 (7)	100.7 (1)	102.93 (6)		
Se-Se-Se-Se(ave., o)	76.2 (3)	76.49 (1)	77.64(10)	78.11 (1)	79.78 (3)	78.5 (2)	77.1 (2)	75.7 (2)	74.6 (1)	65.1 (1)	73.3 (1)		

a) reference [17]; b) reference [34]; c) reference [30]; d) references [35, 36]; e) reference [37]; f) reference [18];

g)

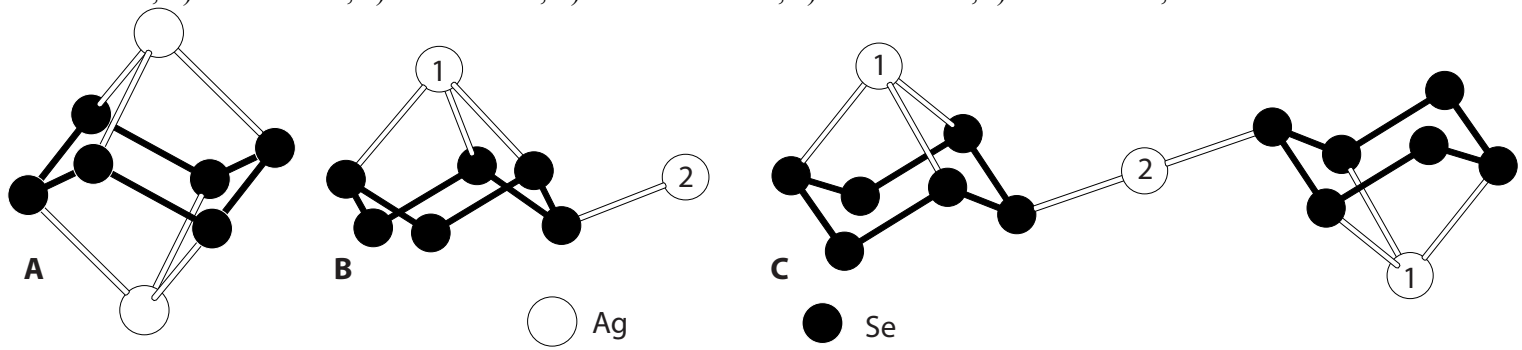
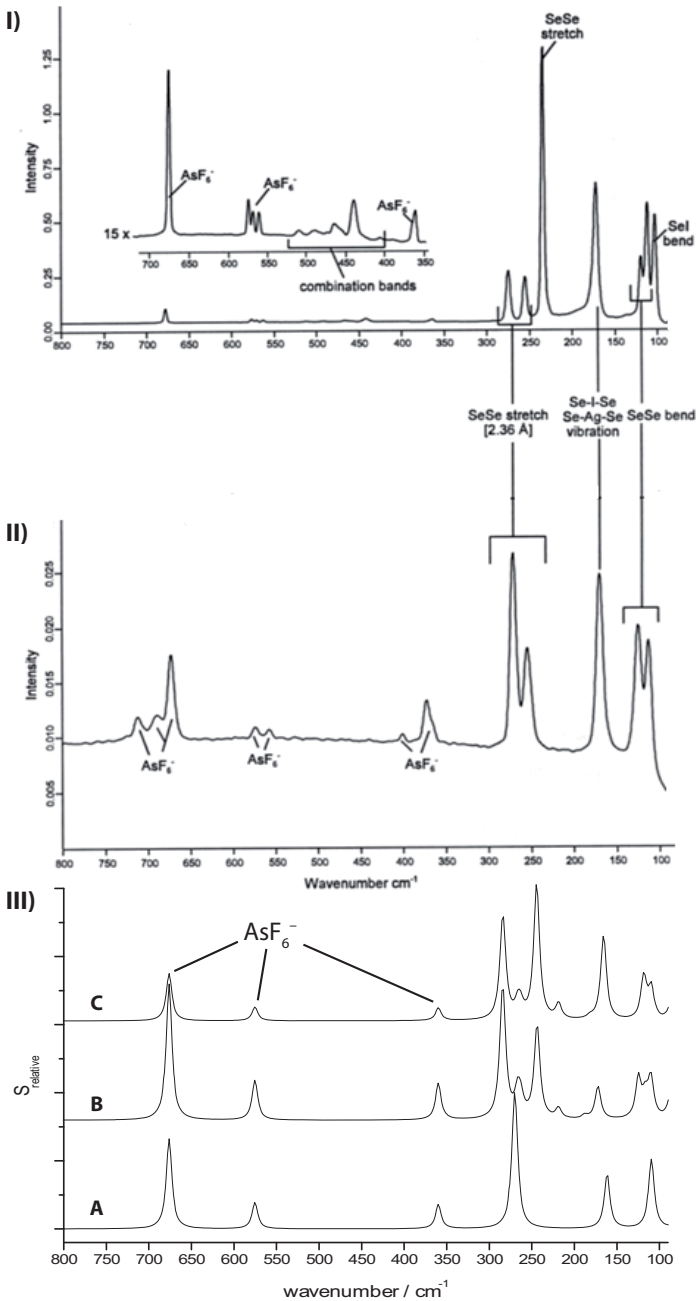


Table S1.6: Comparison of the structural parameters and the strengths [v.u.][43] of the Ag-X (X = Se, O, and F) and Se-F contacts in $[(OSO)AgSe_6Ag(OSO)]^{2+}$ (in **1**), $[(OSO)_2AgSe_6Ag(OSO)_2]^{2+}$ (in **2a**) $[Se_6Ag^+]n$ (in **3**) and $[AgSe_6Ag^{2+}]_n$ (in **4**) and the calculated structures **A**-**E** on pbe0/tzvpp level.

Parameter	**1**	**2**	**3**	**4**	**A**	**B**	**C**	**D**	**E**
d(Ag1-Se) [Å], s[v.u.]	2.885(2), 0.185(3 x)	2.791(3), 0.235(1x)	3.0239(17), 0.127(2 x)	2.9273(18), 0.165(4 x)	2.903	2.756	2.744 (2x)	2.782 (2x)	2.737 (2x)
		2.893(3), 0.179(1x)	3.0636(16), 0.114 (2 x)	2.941(3), 0.158(2 x)		2.929 (2x)	2.946 (4x)	3.009 (2x)	3.046 (2x)
		2.950(3), 0.153(1x)	2.8408(13), 0.208 (2 x)					3.045 (2x)	3.295 (2x)
d(Ag1-Se) (Ave. [Å])	2.885	2.878	2.976	2.932					
Σs(Ag1-Se), s[v.u.]	0.555	0.567	0.898	0.976		2.575	2.581		
d(Ag2-Se) [Å], s[v.u.](in 4)				2.688(3), 0.314 (2 x)					
Σs(Ag2-Se), s[v.u.]				0.628					
d(Ag1-O) [Å], s [v.u.]	2.28(3), 0.310 (1x)	2.362(15), 0.247 (1x)						2.258 (2x)	2.358 (2x)
		2.439(17), 0.199 (1x)							2.489 (2x)
Σs(Ag1-O), s[v.u.]		0.446							
d(Ag1-O') [Å], s[v.u.](in 2)		3.139(1), 0.030 (1x)							
d(Ag1-F) [Å], s[v.u.]	2.988(4), 0.040(3 x)	3.017(2), 0.021(1x)	3.095(1), 0.03 (1 x)						
d(Ag2-F) [Å], s[v.u.](in 4) a				2.689(6), 0.090(4 x)					
				3.053(6), 0.034(4 x)					
d(Se-F)range [Å]	3.170-3.384	3.017	2.912 – 3.218	3.080-3.350					
Σs(Ag1-F), s[v.u.]	0.120 (2 x)		0.03						
Σs(Ag2-F), s[v.u.] (in 4)				0.496					
Σs(Ag1-X), s[v.u.]	0.985	1.064	0.928	0.976					
Σs(Ag2-X), s[v.u.] (in 4)				1.124					

S3 FT Raman Spectra of **4**



I) $(Se_6I)_n n[AsF_6]$(exp. 150K, 5mm glass tube, 5000scans, 2cm^{-1} resolution,11mW laser beam)

II) **4** (exp. R.T., melting point capillaries, 1200 scans, 4cm^{-1} resolution, 18 mW laser beam).

III) Calculated on the PBE0/tzvpp levels **A**, **B** and **C** denote fragments according to Table 1 in the main text.

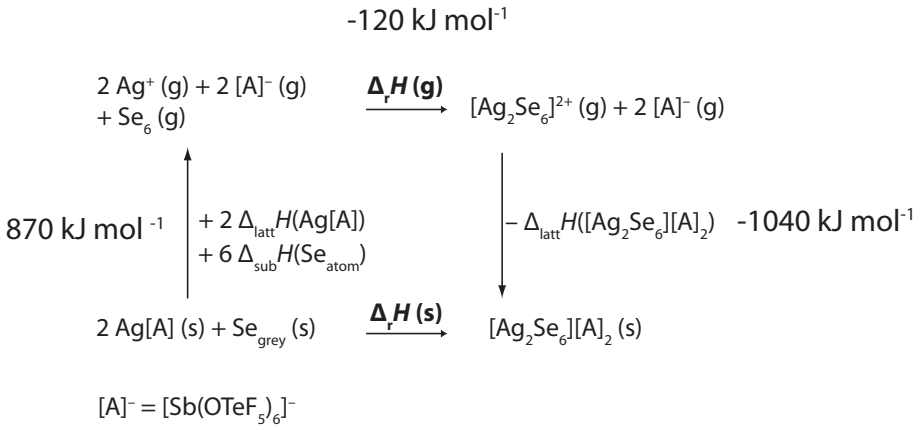
S4 Quantum chemical calculations

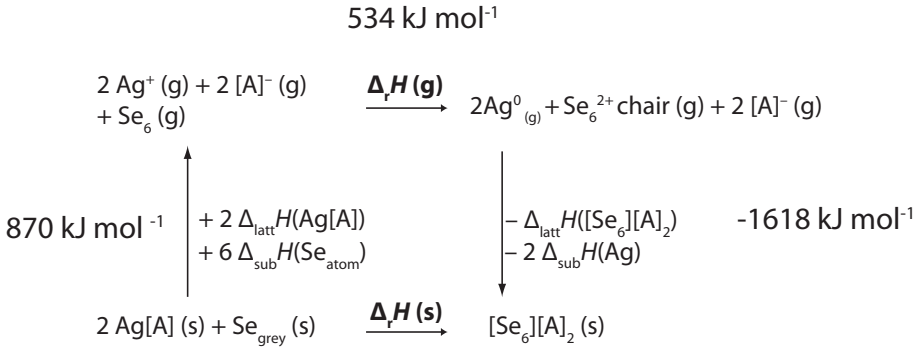
S4.1 Energetics of the calculated compounds

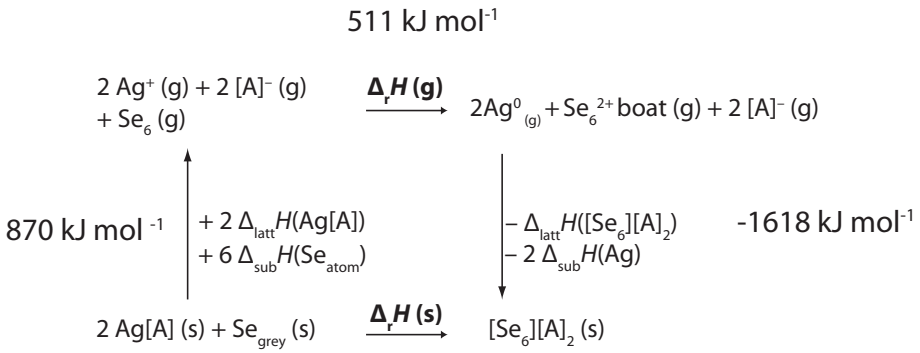
compound	method	basisset	total energy (Hartree)	ZPE (Hartree)	total energy + ZPE (Hartree)	total energy + ZPE (kJ/mol)	enthalpy 298.15 K (kJ/mol)
Ag^{+}	bp	svp	-146.7596727	0	-146.7596727	-385317.509	-385311.3115
Ag^{+}	pbe0	tzvpp	-146.6844728	0	-146.6844728	-385120.0716	-385113.8741
$Ag_2Se_6^{2+}$	bp	svp	-14703.00751	0.0054151	-14703.0021	-38602730.83	-38602688.61
$Ag_2Se_6^{2+}$	pbe0	tzvpp	-14701.16432	0.0061552	-14701.15817	-38597889.59	-38597848.81
Se_6^{2+}_boat	bp	svp	-14408.68031	0.0048117	-14408.6755	-37829976.36	-37829947.23
Se_6^{2+}_boat	pbe0	tzvpp	-14406.99728	0.0054946	-14406.99179	-37825555.78	-37825528.04
Se_6^{2+}_chair	bp	svp	-14408.68116	0.0043771	-14408.67679	-37829979.75	-37829949.82
Se_6^{2+}_chair	pbe0	tzvpp	-14406.98819	0.0050619	-14406.98312	-37825533.04	-37825504.37
Se_8^{2+}	bp	svp	-19211.87721	0.0064039	-19211.8708	-50440765.25	-50440724.93
Se_8^{2+}	pbe0	tzvpp	-19209.62835	0.0073466	-19209.62101	-50434858.42	-50434819.94
Se_6	bp	svp	-14409.42699	0.0044854	-14409.4225	-37831937.63	-37831907.96
Se_6	pbe0	tzvpp	-14407.74854	0.0052028	-14407.74333	-37827528.97	-37827500.67
Ag	bp	svp	-147.0591299	0	-147.0591299	-386103.7339	-386097.5365
Ag	pbe0	tzvpp	-146.930293	0	-146.930293	-385765.4725	-385759.2751
$Ag_2Se_6(SO_2)_2^{2+}$	bp	svp			0	0	2.478968175
$Ag_2Se_6(SO_2)_2^{2+}$	pbe0	tzvpp	-15798.05812	0.0223095	-15798.03581	-41477741.76	-41477675.52
SO_2	bp	svp	-548.4196476	0.0064362	-548.4132114	-1439858.843	-1439848.332
SO_2	pbe0	tzvpp	-548.4112333	0.0072201	-548.4040132	-1439834.693	-1439824.71
$AgSO_2^{+}$	bp	svp	-695.2306906	0.0073497	-695.2233409	-1825308.826	-1825293.234
$AgSO_2^{+}$	pbe0	tzvpp	-695.1352469	0.0081043	-695.1271426	-1825056.257	-1825041.106
$Ag(SO_2)_2^{+}$	bp	svp			0	0	2.478968175
$Ag(SO_2)_2^{+}$	pbe0	tzvpp	-1243.583969	0.0165106	-1243.567458	-3264986.261	-3264959.061
$AgSe_6SO_2^{+}$	bp	svp			0	0	2.478968175
$AgSe_6SO_2^{+}$	pbe0	tzvpp	-15102.95981	0.013837	-15102.94597	-39652783.45	-39652736.34
$AgSe_6^{+}$	bp	svp	-14556.28883	0.0052026	-14556.28363	-38217521.49	-38217486.08
$AgSe_6^{+}$	pbe0	tzvpp	-14554.52527	0.0058344	-14554.51943	-38212889.61	-38212855.42
Se_8	bp	svp	-19212.58706	0.0062727	-19212.58079	-50442629.33	-50442588.78
Se_8	pbe0	tzvpp	-19210.34421	0.0069981	-19210.33721	-50436738.81	-50436699.63
$Ag_2Se_6(SO_2)_4^{2+}$	pbe0	tzvpp	-16894.92007	0.0381615	-16894.88191	-44357511.1	-44357423.83
Ag_2	pbe0	tzvpp	-293.9899614	0.0004115	-293.9895499	-771869.5398	-771859.3212
$Ag(SO_2)_3^{+}$	pbe0	tzvpp	-1792.013727	0.0241167	-1791.98961	-4704868.578	-4704827.638
$AgSe6(SO_2)_2^{+}$	pbe0	tzvpp	-15651.38298	0.0216066	-15651.36137	-41092648.03	-41092587.54

compound	free enthalpy 298.15 (kJ/mol)	freeh energy	freeh entropy	freeh chem. pot.	diel+OC (hartree)	diel+OC (kJ/mol)	diel+Occorrected	free enthalpy solvation
Ag^{+}	-385361.1439	3.71845226 3	0.16713862 3	-43.63496	-0.108216374	-284.12208	-276.19208	-385637.336
Ag^{+}	-385163.7065	3.71845226 3	0.16713862 3	-43.63496	-0.108216543	-284.122525	-276.192525	-385439.899
$Ag_2Se_6^{2+}$	-38602858.47	53.96	0.56969	-113.41	-0.247464417	-649.7178078	-641.7878078	-38603500.25
$Ag_2Se_6^{2+}$	-38598014.87	54.46	0.55698	-109.12	-0.249228936	-654.3505513	-646.4205513	-38598661.29
Se_6^{2+}_boat	-37830084.37	39.28	0.45995	-95.38	-0.268634165	-705.2989785	-697.3689785	-37830781.74
Se_6^{2+}_boat	-37825659.99	39.69	0.44259	-89.79	-0.273260134	-717.4444602	-709.5144602	-37826369.51
Se_6^{2+}_chair	-37830090.95	38.95	0.47336	-99.7	-0.263132172	-690.8534957	-682.9234957	-37830773.87
Se_6^{2+}_chair	-37825642.91	39.48	0.46465	-96.58	-0.264423733	-694.2444909	-686.3144909	-37826329.23
Se_8^{2+}	-50440891.22	54.66	0.55776	-109.16	-0.243323118	-638.8448271	-630.9148271	-50441522.14
Se_8^{2+}	-50434981.03	55.29	0.54031	-103.33	-0.24660319	-647.4566564	-639.5266564	-50435620.56
Se_6	-37832041.44	38.96	0.44769	-92.04	-0.003928146	-10.31334596	-2.383345959	-37832043.83
Se_6	-37827630.79	39.48	0.4364	-88.15	-0.003957287	-10.3898567	-2.459856702	-37827633.24
Ag	-386147.3689	3.71845226 3	0.16713862 3	-43.63496	-3.464E-07	-0.000909473	7.929090527	-386139.4398
Ag	-385809.1075	3.71845226 3	0.16713862 3	-43.63496	-0.000000649	-0.001703949	7.928296051	-385801.1792
$Ag_2Se_6(SO_2)_2^{2+}$	2.478968175					0	7.93	7.93
$Ag_2Se_6(SO_2)_2^{2+}$	-41477941.53	122.33	0.89221	-141.2	-0.222111782	-583.1544667	-575.2244667	-41478516.75
SO_2	-1439922.831	24.93	0.24987	-47.09	-0.006733579	-17.67900981	-9.749009813	-1439932.58
SO_2	-1439898.765	26.46	0.24838	-45.11	-0.007050361	-18.5107225	-10.5807225	-1439909.34
$AgSO_2^{+}$	-1825391.206	32.41	0.3286	-63.09	-0.091543741	-240.3480839	-232.4180839	-1825623.631
$AgSO_2^{+}$	-1825139.338	33.95	0.32947	-61.8	-0.092989886	-244.1449377	-236.2149377	-1825375.55
$Ag(SO_2)_2^{+}$	2.478968175					0	7.93	7.93
$Ag(SO_2)_2^{+}$	-3265100.73	68.07	0.47516	-71.12	-0.081594424	-214.2261524	-206.2961524	-3265307.026
$AgSe_6SO_2^{+}$	2.478968175					0	7.93	7.93
$AgSe_6SO_2^{+}$	-39652934.3	80.96	0.66397	-114.53	-0.067136694	-176.2673853	-168.3373853	-39653102.64
$AgSe_6^{+}$	-38217636.6	46.59	0.50482	-101.44	-0.0690293	-181.2364227	-173.3064227	-38217809.9
$AgSe_6^{+}$	-38213003.1	47.03	0.49533	-98.18	-0.071028649	-186.4857128	-178.5557128	-38213181.66
Se_8	-50442751.71	54.54	0.54649	-105.91	-0.003547455	-9.313843869	-1.383843869	-50442753.09
Se_8	-50436860.09	55.08	0.53821	-102.9	-0.003765823	-9.88716746	-1.95716746	-50436862.04
$Ag_2Se_6(SO_2)_4^{2+}$	-44357746.3	184.98	1.08157	-135.01	-0.204647993	-537.3032903	-529.3732903	-44358275.68
Ag_2	-771933.2147	8.82	0.24784	-62.59	-0.005247062	-13.77616086	-5.846160861	-771939.0563
$Ag(SO_2)_3^{+}$	-4705022.822	101.78	0.65465	-90.92	-0.076978564	-202.1072128	-194.1772128	-4705216.994
$AgSe6(SO_2)_2^{+}$	-41092827.32	114.74	0.80422	-122.56	-0.065766206	-172.6691694	-164.7391694	-41092992.06

S4.2 Born-Fajans-Haber cycles for estimation of lattice enthalpies







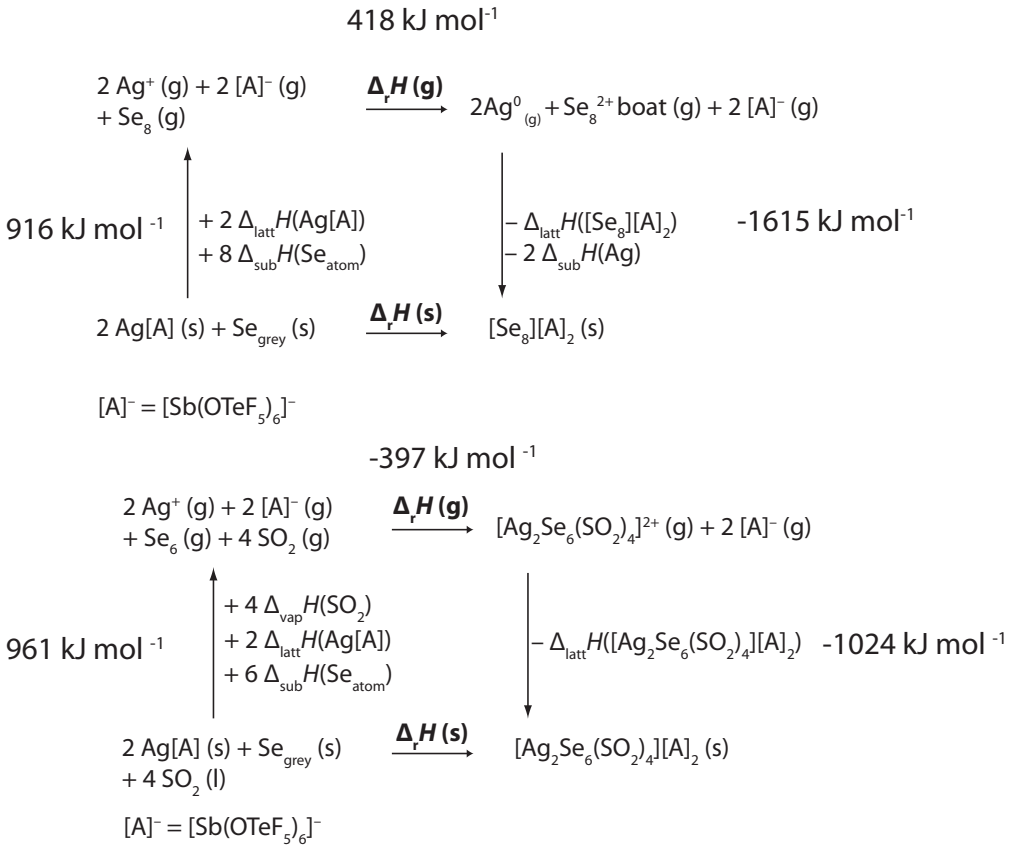


Table S4.2.1: Collected Volumes of Ions used.

Ion	Volume [nm^3]	Origin
$[Sb(OTeF_5)_6]^-$	0.724	Reference[38]
$[Ag_2Se_6]^{2+}$	0.255	Pbe0/tzvpp//cosmo
$[(OSO)AgSe_6Ag(OSO)]^{2+}$	0.308	X-RAY
$[(OSO)_2AgSe_6Ag(OSO)_2]^{2+}$	0.385	X-RAY
Se_6^{2+} chair	0.196	Pbe0/tzvpp/cosmo
Se_6^{2+} boat	0.190	Pbe0/tzvpp/cosmo
Ag+	0.006	Calcd. from Shannon r = 1.15Å[39]
Se_8^{2+}	0.214	Reference[40]

A scaling of the calculated volumes of compound Se_6^{2+} according to reference [41] on the cosmo-pbe0/tzvpp level leads to a change in U_{pot} of 0.4 kJ mol^{-1} and therefore the volumes are used without scaling.

S 4.3 Details of the Quantum Chemical Investigations

S 4.3.1 Calculated Geometries and Spectra PBE0/TZVPP

```
ag2se6_1_pbe0tzvpp
------------------------------------------------------------

$coord
    3.44914832070948      1.99136671143657      0.99561803164237  se
   -3.44914832070948      1.99136671143657      0.99561803164237  se
   -3.44914832070948     -1.99136671143657     -0.99561803164237  se
    3.44914832070948     -1.99136671143657     -0.99561803164237  se
    0.00000000000000      3.98273342287314     -0.99561803164237  se
    0.00000000000000     -3.98273342287314      0.99561803164237  se
    0.00000000000000      0.00000000000000      4.76863270495494  ag
    0.00000000000000      0.00000000000000     -4.76863270495494  ag
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0061552  Hartree  *
         *    SCF-energy                   : -14701.1643206           *
         *    SCF + E(vib0)                : -14701.1581654           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        eu            44.20         0.54081       YES     NO
     8        eu            44.20         0.54081       YES     NO
     9        eg            50.58         0.00000       NO      YES
    10        eg            50.58         0.00000       NO      YES
    11        a1g           77.11         0.00000       NO      YES
    12        a2u           96.93        10.34189       YES     NO
    13        eu           102.17         0.10450       YES     NO
    14        eu           102.17         0.10450       YES     NO
    15        eg           109.52         0.00000       NO      YES
    16        eg           109.52         0.00000       NO      YES
    17        a1g          161.60         0.00000       NO      YES
    18        a2u          178.18         2.85600       YES     NO
    19        a1u          233.31         0.00000       NO      NO
    20        eu           267.60         0.14950       YES     NO
    21        eu           267.60         0.14950       YES     NO
    22        eg           268.16         0.00000       NO      YES
    23        eg           268.16         0.00000       NO      YES
    24        a1g          270.25         0.00000       NO      YES
------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.16797161 H =     +4.57074 eV
------------------------------------------------------------------------
ag2se6_2_pbe0tzvpp
------------------------------------------------------------

$coord
    0.00053683796852      2.74767872767663     -1.73596186641559      se
    3.47939030925524     -3.10235075264850     -1.99580348918949      se
    0.00010657219379     -5.20061866840011     -0.18773876974280      se
   -3.44999885732025      0.64588891946619      0.29578795762287      se
    3.45021012610665      0.64570194230084      0.29674806033669      se
```

```
   -3.47891921689773     -3.10218361441453     -1.99673220304740      se
   -0.00006810122176      7.26280244113295      0.07899936093760      ag
   -0.00090235305042     -1.87103311789480      3.81790780984209      ag
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0061177  Hartree  *
         *    SCF-energy                   : -14701.1579982           *
         *    SCF + E(vib0)                : -14701.1518806           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             27.85         0.27970       YES     YES
     8        a             36.11         0.19262       YES     YES
     9        a             48.54         0.41026       YES     YES
    10        a             57.47         1.57968       YES     YES
    11        a             72.32         1.52061       YES     YES
    12        a             85.13         0.00059       YES     YES
    13        a             88.69         2.61293       YES     YES
    14        a            110.16         0.34428       YES     YES
    15        a            116.83         0.22368       YES     YES
    16        a            124.82         1.51385       YES     YES
    17        a            172.34         2.15631       YES     YES
    18        a            187.87         2.42451       YES     YES
    19        a            218.67         0.22241       YES     YES
    20        a            243.86         3.94238       YES     YES
    21        a            262.67         0.27184       YES     YES
    22        a            266.70         0.11994       YES     YES
    23        a            281.10         0.02470       YES     YES
    24        a            284.23         0.35333       YES     YES
------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                   +0.14333275 H =     +3.90028 eV
--------------------------------------------------------------------------------
ag2se6_3_pbe0tzvpp
------------------------------------------------------------

$coord
   -0.00003164526704      3.76196628175051     -1.46377977650626      se
    3.45857467147156     -1.99827159837028     -0.87801428146664      se
   -0.00000880166699     -3.76197262361926      1.46378270337090      se
   -3.45855801262634      1.99824300713226      0.87807578838537      se
    3.45855580628988      1.99828441048597      0.87802083158133      se
   -3.45854239185286     -1.99825193213670     -0.87806784658176      se
    0.00000727257717      8.38894632953931      0.17429531959179      ag
    0.00000032085515     -8.38894453267594     -0.17430807000524      ag
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0059618  Hartree  *
         *    SCF-energy                   : -14699.3088688           *
         *    SCF + E(vib0)                : -14699.3029069           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
```

```
     1                      0.00         0.00000        -       -
     2                      0.00         0.00000        -       -
     3                      0.00         0.00000        -       -
     4                      0.00         0.00000        -       -
     5                      0.00         0.00000        -       -
     6                      0.00         0.00000        -       -
     7        a            23.01         2.92786      YES     YES
     8        a            31.49         1.90845      YES     YES
     9        a            42.12         0.00000      YES     YES
    10        a            45.76         0.00000      YES     YES
    11        a            71.16         0.00000      YES     YES
    12        a            80.64         0.06075      YES     YES
    13        a            81.43         5.04566      YES     YES
    14        a           100.42         0.00000      YES     YES
    15        a           119.92         5.07066      YES     YES
    16        a           121.83         0.00000      YES     YES
    17        a           182.17         0.00000      YES     YES
    18        a           190.78         7.36530      YES     YES
    19        a           206.50         1.01717      YES     YES
    20        a           236.97         0.00000      YES     YES
    21        a           250.34         4.89854      YES     YES
    22        a           253.58         0.00000      YES     YES
    23        a           286.48         0.59894      YES     YES
    24        a           292.33         0.00000      YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                  +0.13978354 H =     +3.80371 eV
-------------------------------------------------------------------------------
ag2se6_so2_2_pbe0tzvpp
-------------------------------------------------------------

$coord
    2.36148485683856     -3.16516710916646     -0.90577257435874  se
    1.91471553666679      3.62476567925215     -0.16977755562468  se
   -2.36798835436629      3.17062502030217      0.92188538089128  se
   -1.92018425491558     -3.62022968279511      0.18778292248267  se
    2.27973971627730      0.55295369575575     -3.34115776457780  se
   -2.28440832406103     -0.54748205639367      3.35970714419186  se
    3.35764314083208     -0.44957971584814      3.55470015298042  ag
   -3.37630218880326      0.47214076008444     -3.52337866367739  ag
    8.26009866188325     -4.02991522192597      6.92593539859888  o
    7.88138964965738     -1.62976030706722      8.07008603400396  s
    5.97643417749256     -0.01546277302005      6.90929619798684  o
   -5.97360777443634      0.00796030870667     -6.88433642401373  o
   -7.85854716408321      1.60443496822175     -8.10067365309668  s
   -8.25046767898220      4.02471643389369     -7.00429659578688  o
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0223001  Hartree  *
         *    SCF-energy                   : -15798.0579488           *
         *    SCF + E(vib0)                : -15798.0356487           *
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1        a              -6.05         0.00000       YES     YES
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7                       0.00         0.00000        -       -
     8        a              6.33         0.33640       YES     YES
```

```
     9        a              10.96         0.08309       YES     YES
    10        a              14.28         0.01475       YES     YES
    11        a              18.80         1.19987       YES     YES
    12        a              24.00         0.02722       YES     YES
    13        a              25.89         1.39361       YES     YES
    14        a              27.61         0.75242       YES     YES
    15        a              32.72         0.00264       YES     YES
    16        a              35.80         0.00186       YES     YES
    17        a              41.30         0.01717       YES     YES
    18        a              44.63         1.07858       YES     YES
    19        a              75.36         0.00064       YES     YES
    20        a              85.52         7.62148       YES     YES
    21        a              95.56         0.54886       YES     YES
    22        a             103.71         1.44957       YES     YES
    23        a             107.33         0.00001       YES     YES
    24        a             108.31         0.00001       YES     YES
    25        a             156.32         0.00013       YES     YES
    26        a             163.76         9.48712       YES     YES
    27        a             164.85        13.94068       YES     YES
    28        a             174.58         1.02532       YES     YES
    29        a             216.94        27.42302       YES     YES
    30        a             218.70         1.73225       YES     YES
    31        a             236.73         0.03445       YES     YES
    32        a             269.48         0.05068       YES     YES
    33        a             270.02         0.00260       YES     YES
    34        a             271.40         0.00009       YES     YES
    35        a             273.86         0.00525       YES     YES
    36        a             277.01         0.00001       YES     YES
    37        a             543.23        77.11998       YES     YES
    38        a             544.01        19.41765       YES     YES
    39        a            1182.06       421.41932       YES     YES
    40        a            1183.40         4.88638       YES     YES
    41        a            1391.77       461.68956       YES     YES
    42        a            1392.36         0.33185       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.16325607 H =     +4.44243 eV
-------------------------------------------------------------------------------
ag2se6_so2_2_cosmoopt_pbe0_tzvpp
-------------------------------------------------------------

$coord
    1.86160248160618      3.19866531435211     -1.68194287420437  se
    2.00686049913439     -3.51404196669529     -0.45799488229015  se
   -1.86506308099907     -3.20071086221691      1.68114419301817  se
   -2.00981452720006      3.51212456011557      0.45833354944258  se
    3.96562842291913      0.23693930949039      0.86410098948592  se
   -3.96868396261800     -0.23889980901409     -0.86394083596745  se
   -0.16308892677468     -0.82733413209824     -4.68001196172126  ag
    0.16394553256154      0.83217191422887      4.67907344027462  ag
    0.34348213283070      2.28582854574600    -10.79126337312814  o
   -0.11472207104714     -0.34609433329655    -11.14448299882417  s
   -0.36445246540348     -1.86337422630298     -8.88061605441599  o
    0.35537044634356      1.86697974375897      8.88281297709035  o
    0.11342976140206      0.34642392807436     11.14519020542012  s
   -0.32449424275519     -2.28867798614208     10.78959762581974  o
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
```

```
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               3.40         0.02717      YES     YES
     8        a               4.80         0.01982      YES     YES
     9        a               7.75         0.00296      YES     YES
    10        a               9.79         0.41573      YES     YES
    11        a              19.82         1.73323      YES     YES
    12        a              23.20         2.15789      YES     YES
    13        a              25.00         0.00302      YES     YES
    14        a              28.41         0.03219      YES     YES
    15        a              33.74         0.00072      YES     YES
    16        a              35.82         0.00070      YES     YES
    17        a              42.28         0.00011      YES     YES
    18        a              45.90         1.15979      YES     YES
    19        a              77.65         0.00314      YES     YES
    20        a              85.18         7.40548      YES     YES
    21        a              95.88         0.56218      YES     YES
    22        a             106.87         1.42123      YES     YES
    23        a             107.41         0.00038      YES     YES
    24        a             107.99         0.00382      YES     YES
    25        a             157.24         0.00016      YES     YES
    26        a             162.28         5.80531      YES     YES
    27        a             162.67        17.35211      YES     YES
    28        a             174.75         0.96329      YES     YES
    29        a             218.89        27.57086      YES     YES
    30        a             220.50         0.73797      YES     YES
    31        a             237.12         0.04162      YES     YES
    32        a             269.40         0.05100      YES     YES
    33        a             269.82         0.00571      YES     YES
    34        a             271.52         0.00007      YES     YES
    35        a             274.73         0.00582      YES     YES
    36        a             278.32         0.00003      YES     YES
    37        a             543.24        91.30463      YES     YES
    38        a             543.72         3.69708      YES     YES
    39        a            1181.28       432.82428      YES     YES
    40        a            1182.63         1.15636      YES     YES
    41        a            1391.54       461.14812      YES     YES
    42        a            1392.20         9.03841      YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                  +0.14948494 H =     +4.06769 eV
-------------------------------------------------------------------------------
ag2se6_so2_4_pbe0_tzvpp
-------------------------------------------------------------

$coord
    9.68436526893912     -4.92747525726106     -0.74390346028693      s
    8.35229532731317      5.84911366646232      0.07836721313340      s
    8.47398500343425     -2.61351473253212     -1.58194274849897      o
    8.49109229084315     -6.23840772587921      1.28007629356654      o
    8.39430344828057      3.14908826734467      0.48710778034535      o
    5.95963176241307      6.93015115890122     -0.55149714936861      o
    1.52904447141169      0.10755668654391      3.74983871674576      se
    1.12383513358135      3.16746448045698     -2.31036641507338      se
   -0.30582032322738      3.66295512690186      1.83160569909455      se
    5.13224100637098     -0.21145908953699      0.04794438492229      ag
   -1.12102433056916     -3.17687695554074      2.31845949058521      se
   -1.52566387421486     -0.11724407765433     -3.74413261322508      se
   -5.13176171850995      0.21577606447002     -0.05429016953143      ag
    0.30564500025488     -3.67369932492713     -1.82406233830470      se
   -8.46012611128538      2.65129598329077      1.54784407856776      o
   -8.39571002512593     -3.14400134264289     -0.46846987803553      o
```

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   -9.68215758204089      4.95077751035687      0.68681458698494      s
   -8.36431407310235     -5.84063436454799     -0.03649405363596      s
   -8.49914914062949      6.24477480577682     -1.35382402244844      o
   -5.97728700316467     -6.92489865566237      0.60865378697991      o
$end
-------------------------------------------------------------
SCF and ZP-Energy
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1        a              -6.75         0.00000       YES     YES
     2        a              -5.32         0.00000       YES     YES
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7                        0.00         0.00000        -       -
     8                        0.00         0.00000        -       -
     9        a               7.69         0.01896       YES     YES
    10        a               8.40         0.07947       YES     YES
    11        a              12.72         0.79760       YES     YES
    12        a              14.41         0.01298       YES     YES
    13        a              14.87         1.11760       YES     YES
    14        a              18.95         0.61620       YES     YES
    15        a              22.07         0.00131       YES     YES
    16        a              23.81         0.00753       YES     YES
    17        a              24.72         0.02411       YES     YES
    18        a              26.98         1.31421       YES     YES
    19        a              31.98         0.00067       YES     YES
    20        a              35.08         0.00282       YES     YES
    21        a              37.66         0.99368       YES     YES
    22        a              39.91         0.00253       YES     YES
    23        a              44.72         0.92320       YES     YES
    24        a              45.66         0.14373       YES     YES
    25        a              55.99         4.81138       YES     YES
    26        a              56.38         0.00806       YES     YES
    27        a              77.97         0.00625       YES     YES
    28        a              80.21         3.80923       YES     YES
    29        a              93.67         0.46077       YES     YES
    30        a             106.13         0.00003       YES     YES
    31        a             110.35         0.00500       YES     YES
    32        a             110.64         0.04927       YES     YES
    33        a             128.25         0.04638       YES     YES
    34        a             129.68         8.61824       YES     YES
    35        a             135.27         0.96990       YES     YES
    36        a             136.08        20.12476       YES     YES
    37        a             150.19         7.32821       YES     YES
    38        a             151.14        20.16786       YES     YES
    39        a             156.32         0.01320       YES     YES
    40        a             175.04         0.18180       YES     YES
    41        a             188.40        23.10176       YES     YES
    42        a             189.79         0.43015       YES     YES
    43        a             235.65         0.14891       YES     YES
    44        a             265.54         0.00029       YES     YES
    45        a             268.09         0.69892       YES     YES
    46        a             272.10         0.00003       YES     YES
    47        a             278.45         0.10916       YES     YES
    48        a             282.27         0.00002       YES     YES
    49        a             542.17        17.14494       YES     YES
    50        a             542.31        43.74671       YES     YES
    51        a             542.96       175.52744       YES     YES
    52        a             544.71         0.20138       YES     YES
    53        a            1192.84       332.75378       YES     YES
    54        a            1193.27         3.15478       YES     YES
```

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    55        a            1203.05       207.94678       YES     YES
    56        a            1203.96         0.34454       YES     YES
    57        a            1379.09         0.83313       YES     YES
    58        a            1379.98       503.32832       YES     YES
    59        a            1391.49       246.05795       YES     YES
    60        a            1391.95        10.38030       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                   +0.16057755 H =     +4.36954 eV
-------------------------------------------------------------------------------
ag2se6_so2_4_cosmoopt_pbe0_tzvpp
-------------------------------------------------------------

$coord
    9.47090287793709     -4.95301278334396     -0.65402065486008  s
    8.33052090101478      5.82635488579429      0.05931329404041  s
    8.39745076978998     -2.59589795387131     -1.51969944642088  o
    8.15022330537413     -6.23896685709750      1.31500487928301  o
    8.37313513980486      3.11304809036595      0.31566290843826  o
    5.92191745589423      6.96736192043293     -0.38697685987598  o
    1.41810540941003      0.39145080175970      3.75830762539387  se
    1.03585701020313      3.10400162687322     -2.44820947114104  se
   -0.56095288889031      3.72762992753064      1.62472204207591  se
    4.92700932837524     -0.05676696629517     -0.16227284048538  ag
   -1.03300250852191     -3.06766863723910      2.42594149118199  se
   -1.42271356063769     -0.34944985868218     -3.77976712420078  se
   -4.92412687534574      0.07988441660761      0.13956544264008  ag
    0.56000964594452     -3.68750544668444     -1.65019206125818  se
   -8.37473146011004      2.55250259219370      1.64958723226697  o
   -8.36616828048373     -3.08961119166751     -0.41531606449402  o
   -9.47561416151056      4.90425066743062      0.80299996933143  s
   -8.32128476266489     -5.80512888000873     -0.18279155468152  s
   -8.20758120010281      6.18336159128270     -1.20475528606002  o
   -5.91553161450816     -6.94509572106084      0.28062566134268  o
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol         IR     RAMAN
     1        a             -6.75         0.00000       YES     YES
     2        a             -5.32         0.00000       YES     YES
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7                       0.00         0.00000        -       -
     8                       0.00         0.00000        -       -
     9        a              7.69         0.01896       YES     YES
    10        a              8.40         0.07947       YES     YES
    11        a             12.72         0.79760       YES     YES
    12        a             14.41         0.01298       YES     YES
    13        a             14.87         1.11760       YES     YES
    14        a             18.95         0.61620       YES     YES
    15        a             22.07         0.00131       YES     YES
    16        a             23.81         0.00753       YES     YES
    17        a             24.72         0.02411       YES     YES
    18        a             26.98         1.31421       YES     YES
    19        a             31.98         0.00067       YES     YES
    20        a             35.08         0.00282       YES     YES
    21        a             37.66         0.99368       YES     YES
    22        a             39.91         0.00253       YES     YES
    23        a             44.72         0.92320       YES     YES
```

```
    24        a              45.66         0.14373       YES     YES
    25        a              55.99         4.81138       YES     YES
    26        a              56.38         0.00806       YES     YES
    27        a              77.97         0.00625       YES     YES
    28        a              80.21         3.80923       YES     YES
    29        a              93.67         0.46077       YES     YES
    30        a             106.13         0.00003       YES     YES
    31        a             110.35         0.00500       YES     YES
    32        a             110.64         0.04927       YES     YES
    33        a             128.25         0.04638       YES     YES
    34        a             129.68         8.61824       YES     YES
    35        a             135.27         0.96990       YES     YES
    36        a             136.08        20.12476       YES     YES
    37        a             150.19         7.32821       YES     YES
    38        a             151.14        20.16786       YES     YES
    39        a             156.32         0.01320       YES     YES
    40        a             175.04         0.18180       YES     YES
    41        a             188.40        23.10176       YES     YES
    42        a             189.79         0.43015       YES     YES
    43        a             235.65         0.14891       YES     YES
    44        a             265.54         0.00029       YES     YES
    45        a             268.09         0.69892       YES     YES
    46        a             272.10         0.00003       YES     YES
    47        a             278.45         0.10916       YES     YES
    48        a             282.27         0.00002       YES     YES
    49        a             542.17        17.14494       YES     YES
    50        a             542.31        43.74671       YES     YES
    51        a             542.96       175.52744       YES     YES
    52        a             544.71         0.20138       YES     YES
    53        a            1192.84       332.75378       YES     YES
    54        a            1193.27         3.15478       YES     YES
    55        a            1203.05       207.94678       YES     YES
    56        a            1203.96         0.34454       YES     YES
    57        a            1379.09         0.83313       YES     YES
    58        a            1379.98       503.32832       YES     YES
    59        a            1391.49       246.05795       YES     YES
    60        a            1391.95        10.38030       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                  +0.14895074 H =     +4.05316 eV
-------------------------------------------------------------------------------
agse6pbe0_tzvpp
-------------------------------------------------------------

$coord
    2.01328216358389      3.48710699729953     -1.62785968761695  se
    2.01328216358389     -3.48710699729953     -1.62785968761695  se
   -1.96307521405401     -3.40014600982073      0.32365572448021  se
   -1.96307521405401      3.40014600982073      0.32365572448021  se
    3.92615042810803      0.00000000000000      0.32365572448021  se
   -4.02656432716783      0.00000000000000     -1.62785968761695  se
    0.00000000000000      0.00000000000000      3.91261188941022  ag
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0058344  Hartree  *
         *    SCF-energy                   : -14554.5252674           *
         *    SCF + E(vib0)                : -14554.5194329           *
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
```

```
     3                      0.00         0.00000        -       -
     4                      0.00         0.00000        -       -
     5                      0.00         0.00000        -       -
     6                      0.00         0.00000        -       -
     7        e            60.41         0.24934       YES     YES
     8        e            60.41         0.24934       YES     YES
     9        e            91.09         0.13449       YES     YES
    10        e            91.09         0.13449       YES     YES
    11        a1           94.36         3.00542       YES     YES
    12        e           119.17         0.13625       YES     YES
    13        e           119.17         0.13625       YES     YES
    14        a1          144.56         0.09556       YES     YES
    15        a1          184.34         1.32000       YES     YES
    16        a2          231.00         0.00000       NO      NO
    17        e           270.49         0.30476       YES     YES
    18        e           270.49         0.30476       YES     YES
    19        e           274.20         0.53963       YES     YES
    20        e           274.20         0.53963       YES     YES
    21        a1          276.05         0.10615       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                  +0.16802401 H =     +4.57217 eV
-------------------------------------------------------------------------------
agse6_so2_pbe0_tzvpp
-------------------------------------------------------------

$coord
    1.80339887883071      3.29149901399081     -5.15417399517500  se
    2.04993259600390     -3.59854900903202     -4.19858138039336  se
   -1.82007991425296     -3.33351233804769     -2.06698481163009  se
   -2.06858224334775      3.35547143820866     -3.01282077981598  se
    3.90357428128925      0.17398455617372     -2.81566573357424  se
   -4.08721953948624     -0.33065062324477     -4.39610310286127  se
    0.18273133368015      0.56422689268098      1.02533736972357  ag
    0.44783028099243      1.64660231918143      5.26207991983262  o
    0.12436210160159      0.41880104798441      7.68920879338538  s
   -0.53594777531104     -2.18787329789557      7.66770372050840  o
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0138370  Hartree  *
         *    SCF-energy                   : -15102.9598108           *
         *    SCF + E(vib0)                : -15102.9459738           *
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              2.41         0.46834       YES     YES
     8        a             16.46         0.12507       YES     YES
     9        a             22.56         0.71472       YES     YES
    10        a             42.97         0.39951       YES     YES
    11        a             50.14         0.25577       YES     YES
    12        a             51.57         0.21557       YES     YES
    13        a             88.59         3.14477       YES     YES
    14        a             89.89         0.36421       YES     YES
    15        a             90.64         0.38555       YES     YES
    16        a            113.57         0.49475       YES     YES
    17        a            113.91         0.09361       YES     YES
```

```
    18        a              142.70          9.51544       YES     YES
    19        a              143.07          0.11495       YES     YES
    20        a              173.80          1.20581       YES     YES
    21        a              189.92         11.56070       YES     YES
    22        a              233.20          0.00055       YES     YES
    23        a              271.11          0.17720       YES     YES
    24        a              271.69          0.18794       YES     YES
    25        a              276.14          0.69834       YES     YES
    26        a              276.58          0.71243       YES     YES
    27        a              278.96          0.21090       YES     YES
    28        a              539.11         41.98620       YES     YES
    29        a             1196.60        135.98132       YES     YES
    30        a             1398.12        248.16900       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.13271419 H =     +3.61134 eV
-------------------------------------------------------------------------------
agse6_so2_2_pbe0_tzvpp
-------------------------------------------------------------

$coord
   -0.06104590979782      1.53581483177638      5.04921048920667  o
    0.27347039162383     -0.03065217476318      7.25415071656391  s
    0.62189109906828     -2.67609060826551      6.85818016525284  o
   -0.30319223868376      0.65465819763408      0.30707658533112  ag
   -0.83266840761124     -0.88439278456520     -5.07638656749611  se
    3.50966029541405     -0.26242130546455     -5.57839800189195  se
    4.73193780285011     -0.01522240946225     -1.33031188014851  se
    4.56331585002662     -4.21993672967150      0.05219604721831  se
    0.17662918244117     -4.71837070877825      0.38766561965246  se
   -1.11829009189377     -5.11021440003723     -3.82487391773583  se
   -3.17003475731896      4.21628940823359      0.66038335197030  o
   -4.41687567183140      5.92956084524331     -1.06223941532993  s
   -3.97479754428702      5.58097783812030     -3.69665319259320  o
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0216066  Hartree  *
         *    SCF-energy                   : -15651.3829782           *
         *    SCF + E(vib0)                : -15651.3613717           *
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              3.73         0.01302       YES     YES
     8        a             12.06         0.11974       YES     YES
     9        a             16.64         0.07378       YES     YES
    10        a             19.26         0.00888       YES     YES
    11        a             27.55         1.34353       YES     YES
    12        a             29.12         0.29447       YES     YES
    13        a             36.62         0.08091       YES     YES
    14        a             49.22         1.72618       YES     YES
    15        a             50.89         0.44674       YES     YES
    16        a             52.75         1.89392       YES     YES
    17        a             83.99         0.82652       YES     YES
    18        a             86.59         0.36338       YES     YES
    19        a             89.97         0.31064       YES     YES
    20        a            105.20         1.61897       YES     YES
```

```
    21        a             107.96         5.41632       YES     YES
    22        a             113.20         1.74201       YES     YES
    23        a             117.26         2.87596       YES     YES
    24        a             120.46         9.29559       YES     YES
    25        a             141.16         1.52757       YES     YES
    26        a             153.73         9.10607       YES     YES
    27        a             177.85         2.41408       YES     YES
    28        a             234.16         0.00563       YES     YES
    29        a             270.81         0.05853       YES     YES
    30        a             272.90         0.14298       YES     YES
    31        a             276.59         0.80229       YES     YES
    32        a             277.87         0.84601       YES     YES
    33        a             280.91         0.11164       YES     YES
    34        a             537.64        24.96011       YES     YES
    35        a             539.52        81.85859       YES     YES
    36        a            1201.27       115.59533       YES     YES
    37        a            1207.04        86.57893       YES     YES
    38        a            1391.56       350.23577       YES     YES
    39        a            1398.72        27.20642       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.13179158 H =     +3.58623 eV
-------------------------------------------------------------------------------
agso2_pbe0tzvpp
-------------------------------------------------------------

$coord
   -1.43255933352981     -4.00751052065689      0.00000000000000  ag
   -1.60753309381384      0.19966551419585      0.00000000000000  o
    0.22627838872478      2.25904516569991      0.00000000000000  s
    2.81381403861883      1.54879984076113      0.00000000000000  o
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0081043  Hartree  *
         *    SCF-energy                   :   -695.1352469           *
         *    SCF + E(vib0)                :   -695.1271426           *
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a'             46.14         2.88456       YES     YES
     8        a"            162.22        18.52103       YES     YES
     9        a'            231.83         5.49873       YES     YES
    10        a'            541.86        33.13113       YES     YES
    11        a'           1180.54       152.32553       YES     YES
    12        a'           1394.77       211.18907       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.22676672 H =     +6.17064 eV
-------------------------------------------------------------------------------
agso2_2_pbe0tzvpp
-------------------------------------------------------------

$coord
   -0.00008206301681      0.00004058509554     -0.02633267716026  ag
   -0.08515135540008      4.13078934633031     -0.02795411944608  o
    0.08512754055248     -4.13070414864994     -0.02795415771249  o
```

```
    1.78171252490920      6.15525404946446      0.00065929210001  s
   -1.78164237209782     -6.15525599965467      0.00065916391595  s
    4.36136595433189      5.41645769371946      0.04046116492838  o
   -4.36133022927887     -5.41658152630515      0.04046133337450  o
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0165106  Hartree  *
         *    SCF-energy                   :  -1243.5839686           *
         *    SCF + E(vib0)                :  -1243.5674579           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               3.29         0.41052       YES     YES
     8        a              23.88         0.84170       YES     YES
     9        a              42.53         2.82568       YES     YES
    10        a              46.26         0.00969       YES     YES
    11        a              72.50         3.49235       YES     YES
    12        a             155.00         0.00788       YES     YES
    13        a             172.68        29.84483       YES     YES
    14        a             203.16         0.00015       YES     YES
    15        a             279.67         7.27616       YES     YES
    16        a             541.50         0.00214       YES     YES
    17        a             543.70        70.04177       YES     YES
    18        a            1184.23       305.77856       YES     YES
    19        a            1184.63         0.01250       YES     YES
    20        a            1396.56       446.40954       YES     YES
    21        a            1397.74         0.08186       YES     YES
------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                   +0.19773699 H =     +5.38070 eV
--------------------------------------------------------------------------------
agso2_3_pbe0tzvpp
------------------------------------------------------------

$coord
    0.00774060494933     -0.01142921107023      0.88732222863560  ag
    3.84561429677453     -2.13587696385104      1.02696639660071  o
   -0.08332628317468      4.37729097573029      1.03328519793023  o
   -3.76659893498988     -2.25315756343891      1.03711579700945  o
    4.70472339803557     -4.54680535298459      0.04576747710416  s
   -6.27868079904135     -1.77848611878512      0.04875393546817  s
    1.56380651669424      6.33405123178844      0.04792504479485  s
    2.92871663353396     -5.98654004247566     -1.37052707638780  o
   -6.61846030020348      0.47515850896264     -1.37919139260188  o
    3.69646486742177      5.52579453612418     -1.37741760855353  o
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0241167  Hartree  *
         *    SCF-energy                   :  -1792.0137269           *
         *    SCF + E(vib0)                :  -1791.9896102           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
```

```
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               6.31         0.02624       YES     YES
     8        a               6.42         0.02861       YES     YES
     9        a              10.27         0.11972       YES     YES
    10        a              10.56         0.06688       YES     YES
    11        a              11.25         0.10341       YES     YES
    12        a              32.31         2.97875       YES     YES
    13        a              43.18         0.03129       YES     YES
    14        a              44.09         2.66431       YES     YES
    15        a              44.23         2.68397       YES     YES
    16        a             139.91         8.68954       YES     YES
    17        a             140.14         8.77128       YES     YES
    18        a             148.43        27.48237       YES     YES
    19        a             178.96         0.10971       YES     YES
    20        a             185.65         8.22272       YES     YES
    21        a             186.76         8.32365       YES     YES
    22        a             540.86        58.97852       YES     YES
    23        a             540.94        59.42589       YES     YES
    24        a             543.18         4.04592       YES     YES
    25        a            1193.40       174.95926       YES     YES
    26        a            1193.43       173.38537       YES     YES
    27        a            1199.50         8.09388       YES     YES
    28        a            1394.17       266.40357       YES     YES
    29        a            1394.25       267.47234       YES     YES
    30        a            1397.81       155.60470       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.20448138 H =     +5.56422 eV
-------------------------------------------------------------------------------
so2_pbe0_tzvpp
-------------------------------------------------------------

$coord
    0.00000000000000      0.00000000000000     -0.91674937271946  s
   -2.32850100837618      0.00000000000000      0.45837468635970  o
    2.32850100837618      0.00000000000000      0.45837468635970  o
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0072201  Hartree  *
         *    SCF-energy                   :   -548.4112333           *
         *    SCF + E(vib0)                :   -548.4040132           *
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a1             532.09        30.55076       YES     YES
     8        a1            1217.06        32.97101       YES     YES
     9        b1            1420.11       220.72602       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.22678592 H =     +6.17116 eV
-------------------------------------------------------------------------------
```

```
se6_2+_boat_pbe0tzvpp
------------------------------------------------------------

$coord
   -2.08221682044209      2.41981630320981     -1.35707560692137  se
   -2.08231422255380     -2.41973970896652     -1.35706292766456  se
    2.28174536557824      3.12965223531603     -0.77770573455479  se
    2.28162190848369     -3.12974639124949     -0.77769213219229  se
   -3.40907836846912      0.00007350336271      2.09154079719617  se
    3.01024213740299     -0.00005594167254      2.17799560413685  se
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0054946  Hartree  *
         *    SCF-energy                   : -14406.9972798           *
         *    SCF + E(vib0)                : -14406.9917852           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              87.02         1.89721       YES     YES
     8        a              92.43         0.06403       YES     YES
     9        a             115.21         0.49189       YES     YES
    10        a             145.24         1.17915       YES     YES
    11        a             152.38         0.22014       YES     YES
    12        a             165.28         0.15566       YES     YES
    13        a             210.19         0.56141       YES     YES
    14        a             246.44         1.35956       YES     YES
    15        a             262.99         0.25753       YES     YES
    16        a             285.93         0.22544       YES     YES
    17        a             315.53         0.13340       YES     YES
    18        a             333.20         0.64506       YES     YES
------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                   +0.11861008 H =     +3.22755 eV
--------------------------------------------------------------------------------
se6_2+_chair_pbe0tzvpp
------------------------------------------------------------

$coord
    3.63125846781012     -2.09690436516911     -0.57850219319444  se
   -3.63128719386722     -2.09695808210255     -0.57796592067783  se
   -3.63136729103701      2.09691461683495      0.57829888570805  se
    3.63133416385932      2.09685792867280      0.57883455263395  se
    0.00003110978762     -4.19586195682670      0.57817666040822  se
    0.00003074344714      4.19595185859061     -0.57884198487799  se
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0050619  Hartree  *
         *    SCF-energy                   : -14406.9881864           *
         *    SCF + E(vib0)                : -14406.9831245           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
```

```
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              34.12         2.86780       YES     YES
     8        a              35.55         2.86474       YES     YES
     9        a             106.36         0.00000       YES     YES
    10        a             106.38         0.00000       YES     YES
    11        a             125.54         0.00000       YES     YES
    12        a             190.95         0.44787       YES     YES
    13        a             237.64         0.00030       YES     YES
    14        a             252.70         0.00000       YES     YES
    15        a             273.86         0.28381       YES     YES
    16        a             275.55         0.28451       YES     YES
    17        a             290.65         0.00000       YES     YES
    18        a             292.63         0.00000       YES     YES
-------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                    +0.09032298 H =     +2.45781 eV
-------------------------------------------------------------------------------
se8_2+_pbe0tzvpp
-------------------------------------------------------------

$coord
   -2.14657692974305     -0.12357711468802     -2.77215000467083  se
    1.28317746386817     -2.83205419907150     -3.13118703230046  se
   -0.41741026823280      3.89845519206863     -3.18641627981269  se
   -0.04493003904956     -5.62225495537990      0.00000000000000  se
    1.28317746386817     -2.83205419907150      3.13118703230046  se
   -2.14657692974305     -0.12357711468802      2.77215000467083  se
   -0.41741026823280      3.89845519206863      3.18641627981269  se
    2.60654950726488      3.73660719876167      0.00000000000000  se
$user-defined bonds
$end
-------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0073466  Hartree  *
         *    SCF-energy                   : -19209.6283545            *
         *    SCF + E(vib0)                : -19209.6210079            *
-------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a"             45.04         0.20520       YES     YES
     8        a'             55.84         0.56366       YES     YES
     9        a'             83.00         0.11519       YES     YES
    10        a"             88.61         0.00173       YES     YES
    11        a'             98.16         4.94348       YES     YES
    12        a"             99.17         0.00282       YES     YES
    13        a'            115.59         0.17507       YES     YES
    14        a'            129.37         0.14750       YES     YES
    15        a"            152.37         0.14071       YES     YES
    16        a'            152.52         0.08123       YES     YES
    17        a"            217.31         0.09758       YES     YES
    18        a"            241.81         0.00444       YES     YES
    19        a'            265.91         1.94916       YES     YES
    20        a"            282.10         0.06179       YES     YES
    21        a'            283.57         0.43466       YES     YES
```

```
    22        a"            300.75         0.31113       YES     YES
    23        a'            300.95         0.00003       YES     YES
    24        a'            312.69         0.13104       YES     YES
------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                   +0.09721376 H =     +2.64532 eV
--------------------------------------------------------------------------------
se8_pbe0tzvpp
------------------------------------------------------------

$coord
    1.91200403889871      4.61598608202144      1.08598787782985  se
    1.91200403889871     -4.61598608202144     -1.08598787782985  se
   -4.61598608202144      1.91200403889871      1.08598787782985  se
   -4.61598608202144     -1.91200403889871     -1.08598787782985  se
   -1.91200403889871      4.61598608202144     -1.08598787782985  se
    4.61598608202144     -1.91200403889871      1.08598787782985  se
    4.61598608202144      1.91200403889871     -1.08598787782985  se
   -1.91200403889871     -4.61598608202144      1.08598787782985  se
$user-defined bonds
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0069981  Hartree  *
         *    SCF-energy                   : -19210.3442091           *
         *    SCF + E(vib0)                : -19210.3372110           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        e2            36.90         0.00000       NO      YES
     8        e2            36.90         0.00000       NO      YES
     9        e2            74.17         0.00000       NO      YES
    10        e2            74.17         0.00000       NO      YES
    11        e1            96.58         1.18162       YES     NO
    12        e1            96.58         1.18162       YES     NO
    13        a1           109.95         0.00000       NO      YES
    14        b2           119.14         0.50378       YES     NO
    15        e3           124.32         0.00000       NO      YES
    16        e3           124.32         0.00000       NO      YES
    17        b1           252.41         0.00000       NO      NO
    18        e3           263.69         0.00000       NO      YES
    19        e3           263.69         0.00000       NO      YES
    20        e1           278.81         1.71304       YES     NO
    21        e1           278.81         1.71304       YES     NO
    22        a1           279.42         0.00000       NO      YES
    23        e2           280.97         0.00000       NO      YES
    24        e2           280.97         0.00000       NO      YES
------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                   +0.16541460 H =     +4.50116 eV
--------------------------------------------------------------------------------
se6_pbe0tzvpp
------------------------------------------------------------

$coord
    3.41596475639717     -1.97220817164818     -0.99031463448427      se
   -3.41596475639716     -1.97220817164818     -0.99031463448427      se
   -3.41596475639716      1.97220817164818      0.99031463448427      se
```

```
    3.41596475639717      1.97220817164818      0.99031463448427      se
    0.00000000000000     -3.94441634329635      0.99031463448427      se
    0.00000000000000      3.94441634329635     -0.99031463448427      se
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0052028  Hartree  *
         *    SCF-energy                   : -14407.7485374           *
         *    SCF + E(vib0)                : -14407.7433345           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        eu             81.92         0.22858       YES     NO
     8        eu             81.92         0.22858       YES     NO
     9        eg            101.46         0.00000       NO      YES
    10        eg            101.46         0.00000       NO      YES
    11        a1g           134.55         0.00000       NO      YES
    12        a2u           157.22         0.12040       YES     NO
    13        a1u           235.79         0.00000       NO      NO
    14        eg            272.24         0.00000       NO      YES
    15        eg            272.24         0.00000       NO      YES
    16        eu            279.37         2.01254       YES     NO
    17        eu            279.37         2.01254       YES     NO
    18        a1g           286.25         0.00000       NO      YES
------------------------------------------------------------
HOMO-LUMO Gap
   Gap :                   +0.15831980 H =     +4.30810 eV
```

```
ag3se6_2_pbe0tzvpp
------------------------------------------------------------

$coord
   -4.58608472476816     -1.65784546438280      0.00000000000000      se
   12.58149741021154      0.27220843919987      0.00000000000000      se
  -10.43850245800284     -2.03113808852881      3.47957002063485      se
    6.73507343421790     -0.33438183771069      3.44056284544297      se
  -12.58149741021154     -0.27220843919987      0.00000000000000      se
    4.58608472476816      1.65784546438280      0.00000000000000      se
   -6.73507343421790      0.33438183771070     -3.44056284544297      se
   10.43850245800284      2.03113808852881     -3.47957002063485      se
   -6.73507343421790      0.33438183771070      3.44056284544297      se
   10.43850245800284      2.03113808852881      3.47957002063485      se
  -10.43850245800284     -2.03113808852881     -3.47957002063485      se
    6.73507343421790     -0.33438183771069     -3.44056284544297      se
    0.00000000000000      0.00000000000000      0.00000000000000      ag
   -9.38874861283560      3.81464125421326      0.00000000000000      ag
    9.38874861283560     -3.81464125421326      0.00000000000000      ag
$end
------------------------------------------------------------
SCF and ZP-Energy
         *  zero point VIBRATIONAL energy  :      0.0122686  Hartree  *
         *    SCF-energy                   : -29255.5930513           *
         *    SCF + E(vib0)                : -29255.5807827           *
------------------------------------------------------------
Vibrational Spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
```

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	au	3.62	0.17852	YES	NO
8	au	6.67	0.09790	YES	NO
9	bu	6.91	0.24268	YES	NO
10	ag	17.59	0.00000	NO	YES
11	bg	26.26	0.00000	NO	YES
12	ag	38.60	0.00000	NO	YES
13	bu	41.12	0.93158	YES	NO
14	au	44.11	0.45432	YES	NO
15	bg	45.66	0.00000	NO	YES
16	ag	55.68	0.00000	NO	YES
17	au	62.17	0.00633	YES	NO
18	bu	63.68	2.01476	YES	NO
19	bu	84.22	0.32458	YES	NO
20	bg	85.54	0.00000	NO	YES
21	au	85.74	0.01690	YES	NO
22	ag	88.39	0.00000	NO	YES
23	bu	89.17	5.09804	YES	NO
24	bg	109.61	0.00000	NO	YES
25	au	109.88	1.11794	YES	NO
26	ag	116.28	0.00000	NO	YES
27	ag	118.60	0.00000	NO	YES
28	bu	119.05	0.30035	YES	NO
29	bu	130.70	1.59619	YES	NO
30	ag	165.81	0.00000	NO	YES
31	bu	174.94	4.38169	YES	NO
32	ag	181.69	0.00000	NO	YES
33	bu	198.62	4.47297	YES	NO
34	bg	218.49	0.00000	NO	YES
35	au	219.93	0.24666	YES	NO
36	bu	242.95	19.12701	YES	NO
37	ag	244.38	0.00000	NO	YES
38	bg	262.79	0.00000	NO	YES
39	au	263.30	0.50985	YES	NO
40	ag	266.39	0.00000	NO	YES
41	bu	266.44	0.22759	YES	NO
42	bg	280.91	0.00000	NO	YES
43	au	281.12	0.07659	YES	NO
44	ag	284.09	0.00000	NO	YES
45	bu	284.18	1.01866	YES	NO

HOMO-LUMO Gap
Gap : +0.14625249 H = +3.97974 eV

S 4.3.2 Bond Analysis

$Ag_2Se_6(SO_2)_4^{2+}$ **(2)**

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 1.0 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
1. BD (1) S 1 - O 3	/284. RY*(2) O 4	1.21	1.96	0.044
1. BD (1) S 1 - O 3	/796. BD*(2) S 1 - O 3	22.02	1.10	0.143
1. BD (1) S 1 - O 3	/797. BD*(1) S 1 - O 4	19.96	1.07	0.133
2. BD (2) S 1 - O 3	/284. RY*(2) O 4	2.61	1.66	0.061
2. BD (2) S 1 - O 3	/300. RY*(18) O 4	2.17	2.17	0.063
2. BD (2) S 1 - O 3	/795. BD*(1) S 1 - O 3	19.14	0.82	0.113
2. BD (2) S 1 - O 3	/796. BD*(2) S 1 - O 3	2.21	0.80	0.038

```
  2. BD (   2) S   1 - O   3        /797. BD*(   1) S   1 - O   4          47.95    0.78    0.173
  2. BD (   2) S   1 - O   3        /798. BD*(   2) S   1 - O   4           1.84    0.88    0.036
  3. BD (   1) S   1 - O   4        /259. RY*(   3) O   3                   2.52    1.20    0.051
  3. BD (   1) S   1 - O   4        /263. RY*(   7) O   3                   1.81    2.14    0.058
  3. BD (   1) S   1 - O   4        /274. RY*(  18) O   3                   1.01    2.40    0.046
  3. BD (   1) S   1 - O   4        /284. RY*(   2) O   4                   1.48    1.52    0.044
  3. BD (   1) S   1 - O   4        /300. RY*(  18) O   4                   1.11    2.02    0.044
  3. BD (   1) S   1 - O   4        /795. BD*(   1) S   1 - O   3          19.93    0.68    0.104
  3. BD (   1) S   1 - O   4        /796. BD*(   2) S   1 - O   3          61.34    0.66    0.180
  3. BD (   1) S   1 - O   4        /797. BD*(   1) S   1 - O   4          16.39    0.63    0.091
  3. BD (   1) S   1 - O   4        /798. BD*(   2) S   1 - O   4           1.15    0.73    0.026
  4. BD (   2) S   1 - O   4        /796. BD*(   2) S   1 - O   3           3.07    1.27    0.058
  4. BD (   2) S   1 - O   4        /797. BD*(   1) S   1 - O   4           1.28    1.25    0.037
 34. CR (   1) O   4                /194. RY*(   2) S   1                   1.25   19.92    0.142
 34. CR (   1) O   4                /195. RY*(   3) S   1                   1.01   20.65    0.129
145. LP (   1) O   3                /196. RY*(   4) S   1                   3.20    2.36    0.079
145. LP (   1) O   3                /798. BD*(   2) S   1 - O   4           1.54    1.21    0.039
146. LP (   2) O   3                /193. RY*(   1) S   1                  11.34    1.03    0.098
146. LP (   2) O   3                /194. RY*(   2) S   1                   3.46    1.27    0.061
146. LP (   2) O   3                /798. BD*(   2) S   1 - O   4          17.64    0.73    0.103
147. LP (   1) O   4                /195. RY*(   3) S   1                   4.25    2.47    0.092
148. LP (   2) O   4                /193. RY*(   1) S   1                  20.35    0.99    0.130
148. LP (   2) O   4                /795. BD*(   1) S   1 - O   3          19.65    0.64    0.101
148. LP (   2) O   4                /796. BD*(   2) S   1 - O   3           7.64    0.62    0.061
795. BD*(   1) S   1 - O   3        /193. RY*(   1) S   1                  10.27    0.36    0.168
795. BD*(   1) S   1 - O   3        /194. RY*(   2) S   1                   9.08    0.59    0.227
795. BD*(   1) S   1 - O   3        /260. RY*(   4) O   3                   1.02    1.11    0.116
795. BD*(   1) S   1 - O   3        /798. BD*(   2) S   1 - O   4           1.65    0.06    0.026
796. BD*(   2) S   1 - O   3        /193. RY*(   1) S   1                   3.99    0.38    0.101
796. BD*(   2) S   1 - O   3        /194. RY*(   2) S   1                   3.55    0.62    0.133
796. BD*(   2) S   1 - O   3        /198. RY*(   6) S   1                   1.41    0.59    0.090
796. BD*(   2) S   1 - O   3        /259. RY*(   3) O   3                   1.78    0.54    0.096
796. BD*(   2) S   1 - O   3        /263. RY*(   7) O   3                   1.32    1.48    0.138
796. BD*(   2) S   1 - O   3        /284. RY*(   2) O   4                   1.79    0.86    0.122
796. BD*(   2) S   1 - O   3        /300. RY*(  18) O   4                   1.04    1.37    0.117
796. BD*(   2) S   1 - O   3        /795. BD*(   1) S   1 - O   3           1.54    0.02    0.013
796. BD*(   2) S   1 - O   3        /798. BD*(   2) S   1 - O   4           8.47    0.08    0.064
797. BD*(   1) S   1 - O   4        /218. RY*(  26) S   1                   1.06    2.00    0.157
797. BD*(   1) S   1 - O   4        /259. RY*(   3) O   3                   1.34    0.56    0.094
797. BD*(   1) S   1 - O   4        /284. RY*(   2) O   4                   1.77    0.88    0.135
797. BD*(   1) S   1 - O   4        /300. RY*(  18) O   4                   2.85    1.39    0.215
797. BD*(   1) S   1 - O   4        /795. BD*(   1) S   1 - O   3         123.02    0.04    0.178
797. BD*(   1) S   1 - O   4        /796. BD*(   2) S   1 - O   3         770.44    0.02    0.305
  1. BD (   1) S   1 - O   3        /165. LP*(   7)Ag  10                   2.89    0.90    0.046
  2. BD (   2) S   1 - O   3        /165. LP*(   7)Ag  10                   1.14    0.60    0.023
  4. BD (   2) S   1 - O   4        /165. LP*(   7)Ag  10                   1.30    1.07    0.034
 24. CR (   2) S   1                /165. LP*(   7)Ag  10                   4.20    9.39    0.182
 33. CR (   1) O   3                /165. LP*(   7)Ag  10                   2.23   19.14    0.189
143. LP (   1) S   1                /164. LP*(   6)Ag  10                   1.01    0.61    0.024
143. LP (   1) S   1                /165. LP*(   7)Ag  10                   9.38    0.73    0.075
145. LP (   1) O   3                /164. LP*(   6)Ag  10                   5.96    0.82    0.066
145. LP (   1) O   3                /165. LP*(   7)Ag  10                  12.63    0.94    0.098
145. LP (   1) O   3                /166. LP*(   8)Ag  10                   1.69    0.93    0.036
145. LP (   1) O   3                /167. LP*(   9)Ag  10                   1.37    0.92    0.032
146. LP (   2) O   3                /164. LP*(   6)Ag  10                   5.33    0.33    0.039
146. LP (   2) O   3                /165. LP*(   7)Ag  10                   2.78    0.45    0.032
147. LP (   1) O   4                /165. LP*(   7)Ag  10                   2.81    0.93    0.047
  5. BD (   1) S   2 - O   5        /800. BD*(   2) S   2 - O   5          24.41    1.04    0.145
  5. BD (   1) S   2 - O   5        /801. BD*(   1) S   2 - O   6          27.62    1.01    0.152
  6. BD (   2) S   2 - O   5        /337. RY*(   3) O   6                   2.50    1.68    0.059
  6. BD (   2) S   2 - O   5        /342. RY*(   8) O   6                   1.53    2.33    0.055
  6. BD (   2) S   2 - O   5        /799. BD*(   1) S   2 - O   5          22.85    0.88    0.128
  6. BD (   2) S   2 - O   5        /800. BD*(   2) S   2 - O   5           1.01    0.86    0.027
  6. BD (   2) S   2 - O   5        /801. BD*(   1) S   2 - O   6          40.39    0.84    0.166
  6. BD (   2) S   2 - O   5        /802. BD*(   2) S   2 - O   6           3.68    0.92    0.052
  7. BD (   1) S   2 - O   6        /253. RY*(  29) S   2                   1.25    2.66    0.053
  7. BD (   1) S   2 - O   6        /311. RY*(   3) O   5                   2.63    1.31    0.054
  7. BD (   1) S   2 - O   6        /315. RY*(   7) O   5                   1.09    2.36    0.047
  7. BD (   1) S   2 - O   6        /316. RY*(   8) O   5                   1.05    2.27    0.045
  7. BD (   1) S   2 - O   6        /322. RY*(  14) O   5                   1.21    2.11    0.047
  7. BD (   1) S   2 - O   6        /337. RY*(   3) O   6                   1.29    1.50    0.041
  7. BD (   1) S   2 - O   6        /799. BD*(   1) S   2 - O   5          27.43    0.70    0.124
  7. BD (   1) S   2 - O   6        /800. BD*(   2) S   2 - O   5          45.29    0.68    0.157
  7. BD (   1) S   2 - O   6        /801. BD*(   1) S   2 - O   6          13.31    0.65    0.083
  7. BD (   1) S   2 - O   6        /802. BD*(   2) S   2 - O   6           3.09    0.74    0.043
  8. BD (   2) S   2 - O   6        /800. BD*(   2) S   2 - O   5           5.23    1.26    0.075
  8. BD (   2) S   2 - O   6        /801. BD*(   1) S   2 - O   6           3.48    1.23    0.060
 36. CR (   1) O   6                /226. RY*(   2) S   2                   1.17   19.93    0.138
149. LP (   1) O   5                /228. RY*(   4) S   2                   3.34    2.36    0.080
149. LP (   1) O   5                /802. BD*(   2) S   2 - O   6           1.08    1.20    0.033
150. LP (   2) O   5                /225. RY*(   1) S   2                  13.22    1.00    0.105
150. LP (   2) O   5                /226. RY*(   2) S   2                   3.02    1.26    0.057
```

150. LP (2) O 5	/801. BD*(1) S 2 - O 6	1.07	0.62	0.023
150. LP (2) O 5	/802. BD*(2) S 2 - O 6	19.17	0.70	0.105
151. LP (1) O 6	/227. RY*(3) S 2	4.38	2.59	0.095
152. LP (2) O 6	/225. RY*(1) S 2	18.90	0.99	0.125
152. LP (2) O 6	/226. RY*(2) S 2	1.28	1.24	0.037
152. LP (2) O 6	/799. BD*(1) S 2 - O 5	16.58	0.64	0.093
152. LP (2) O 6	/800. BD*(2) S 2 - O 5	10.02	0.63	0.071
799. BD*(1) S 2 - O 5	/225. RY*(1) S 2	7.47	0.34	0.140
799. BD*(1) S 2 - O 5	/226. RY*(2) S 2	9.04	0.60	0.226
800. BD*(2) S 2 - O 5	/225. RY*(1) S 2	4.47	0.36	0.107
800. BD*(2) S 2 - O 5	/226. RY*(2) S 2	5.38	0.61	0.168
800. BD*(2) S 2 - O 5	/230. RY*(6) S 2	2.06	0.30	0.081
800. BD*(2) S 2 - O 5	/253. RY*(29) S 2	1.19	1.98	0.157
800. BD*(2) S 2 - O 5	/311. RY*(3) O 5	1.35	0.63	0.094
800. BD*(2) S 2 - O 5	/322. RY*(14) O 5	1.07	1.43	0.127
800. BD*(2) S 2 - O 5	/337. RY*(3) O 6	1.26	0.82	0.103
800. BD*(2) S 2 - O 5	/799. BD*(1) S 2 - O 5	4.91	0.02	0.021
800. BD*(2) S 2 - O 5	/802. BD*(2) S 2 - O 6	20.62	0.06	0.086
801. BD*(1) S 2 - O 6	/230. RY*(6) S 2	1.82	0.33	0.082
801. BD*(1) S 2 - O 6	/253. RY*(29) S 2	1.12	2.00	0.157
801. BD*(1) S 2 - O 6	/311. RY*(3) O 5	1.48	0.66	0.103
801. BD*(1) S 2 - O 6	/337. RY*(3) O 6	1.39	0.84	0.113
801. BD*(1) S 2 - O 6	/342. RY*(8) O 6	1.38	1.49	0.151
801. BD*(1) S 2 - O 6	/799. BD*(1) S 2 - O 5	191.52	0.04	0.213
801. BD*(1) S 2 - O 6	/800. BD*(2) S 2 - O 5	549.77	0.02	0.271
5. BD (1) S 2 - O 5	/166. LP*(8)Ag 10	3.37	0.83	0.047
6. BD (2) S 2 - O 5	/166. LP*(8)Ag 10	1.79	0.66	0.031
29. CR (2) S 2	/166. LP*(8)Ag 10	3.14	9.38	0.157
35. CR (1) O 5	/166. LP*(8)Ag 10	2.27	19.13	0.190
144. LP (1) S 2	/164. LP*(6)Ag 10	1.17	0.61	0.025
144. LP (1) S 2	/166. LP*(8)Ag 10	7.03	0.73	0.065
149. LP (1) O 5	/164. LP*(6)Ag 10	4.54	0.82	0.058
149. LP (1) O 5	/166. LP*(8)Ag 10	14.86	0.93	0.106
150. LP (2) O 5	/164. LP*(6)Ag 10	3.05	0.32	0.029
150. LP (2) O 5	/166. LP*(8)Ag 10	1.76	0.44	0.025
151. LP (1) O 6	/165. LP*(7)Ag 10	1.05	0.93	0.029
151. LP (1) O 6	/166. LP*(8)Ag 10	1.31	0.93	0.032
153. LP (1)Se 7	/805. BD*(1)Se 8 -Se 9	1.07	0.72	0.025
153. LP (1)Se 7	/807. BD*(1)Se 11 -Se 14	1.13	0.72	0.026
154. LP (2)Se 7	/368. RY*(8)Se 7	1.53	1.23	0.040
154. LP (2)Se 7	/805. BD*(1)Se 8 -Se 9	1.97	0.34	0.024
154. LP (2)Se 7	/807. BD*(1)Se 11 -Se 14	1.95	0.34	0.024
156. LP (2)Se 8	/421. RY*(1)Se 9	1.30	0.87	0.031
156. LP (2)Se 8	/803. BD*(1)Se 7 -Se 9	3.84	0.28	0.030
156. LP (2)Se 8	/808. BD*(1)Se 12 -Se 14	3.63	0.28	0.029
158. LP (2)Se 9	/361. RY*(1)Se 7	1.45	0.78	0.031
158. LP (2)Se 9	/391. RY*(1)Se 8	1.55	0.82	0.033
158. LP (2)Se 9	/804. BD*(1)Se 7 -Se 11	5.13	0.25	0.032
158. LP (2)Se 9	/806. BD*(1)Se 8 -Se 12	5.56	0.25	0.033
169. LP (2)Se 11	/597. RY*(1)Se 14	1.31	0.87	0.031
169. LP (2)Se 11	/803. BD*(1)Se 7 -Se 9	3.68	0.28	0.029
169. LP (2)Se 11	/808. BD*(1)Se 12 -Se 14	3.90	0.28	0.030
170. LP (1)Se 12	/805. BD*(1)Se 8 -Se 9	1.13	0.72	0.026
170. LP (1)Se 12	/807. BD*(1)Se 11 -Se 14	1.08	0.72	0.025
171. LP (2)Se 12	/531. RY*(8)Se 12	1.55	1.23	0.041
171. LP (2)Se 12	/805. BD*(1)Se 8 -Se 9	1.94	0.34	0.024
171. LP (2)Se 12	/807. BD*(1)Se 11 -Se 14	1.96	0.34	0.024
182. LP (2)Se 14	/494. RY*(1)Se 11	1.54	0.82	0.033
182. LP (2)Se 14	/524. RY*(1)Se 12	1.46	0.78	0.031
182. LP (2)Se 14	/804. BD*(1)Se 7 -Se 11	5.57	0.25	0.033
182. LP (2)Se 14	/806. BD*(1)Se 8 -Se 12	5.15	0.25	0.032
804. BD*(1)Se 7 -Se 11	/807. BD*(1)Se 11 -Se 14	1.98	0.01	0.014
806. BD*(1)Se 8 -Se 12	/805. BD*(1)Se 8 -Se 9	1.95	0.01	0.014
9. BD (1)Se 7 -Se 9	/164. LP*(6)Ag 10	3.07	0.50	0.038
9. BD (1)Se 7 -Se 9	/165. LP*(7)Ag 10	3.42	0.62	0.042
9. BD (1)Se 7 -Se 9	/167. LP*(9)Ag 10	1.34	0.60	0.026
10. BD (1)Se 7 -Se 11	/164. LP*(6)Ag 10	2.25	0.50	0.032
10. BD (1)Se 7 -Se 11	/165. LP*(7)Ag 10	1.27	0.62	0.026
10. BD (1)Se 7 -Se 11	/166. LP*(8)Ag 10	2.33	0.62	0.034
10. BD (1)Se 7 -Se 11	/167. LP*(9)Ag 10	1.47	0.60	0.027
11. BD (1)Se 8 -Se 9	/164. LP*(6)Ag 10	2.61	0.50	0.035
11. BD (1)Se 8 -Se 9	/165. LP*(7)Ag 10	4.77	0.62	0.050
12. BD (1)Se 8 -Se 12	/164. LP*(6)Ag 10	1.25	0.50	0.024
12. BD (1)Se 8 -Se 12	/165. LP*(7)Ag 10	2.10	0.62	0.033
12. BD (1)Se 8 -Se 12	/167. LP*(9)Ag 10	1.04	0.60	0.023
13. BD (1)Se 11 -Se 14	/164. LP*(6)Ag 10	1.43	0.50	0.026
13. BD (1)Se 11 -Se 14	/166. LP*(8)Ag 10	3.49	0.62	0.042
14. BD (1)Se 12 -Se 14	/164. LP*(6)Ag 10	1.04	0.50	0.022
14. BD (1)Se 12 -Se 14	/166. LP*(8)Ag 10	2.34	0.62	0.035
39. CR (3)Se 7	/164. LP*(6)Ag 10	5.87	10.72	0.241
39. CR (3)Se 7	/165. LP*(7)Ag 10	3.10	10.84	0.168
39. CR (3)Se 7	/166. LP*(8)Ag 10	2.07	10.83	0.137

39. CR (3)Se 7	/167. LP*(9)Ag 10	5.44	10.82	0.219
53. CR (3)Se 8	/164. LP*(6)Ag 10	3.55	10.66	0.187
53. CR (3)Se 8	/165. LP*(7)Ag 10	5.87	10.78	0.230
53. CR (3)Se 8	/167. LP*(9)Ag 10	2.23	10.76	0.140
67. CR (3)Se 9	/164. LP*(6)Ag 10	1.26	10.61	0.111
67. CR (3)Se 9	/165. LP*(7)Ag 10	3.00	10.73	0.164
85. CR (3)Se 11	/166. LP*(8)Ag 10	1.78	10.77	0.126
117. CR (3)Se 14	/164. LP*(6)Ag 10	2.21	10.61	0.147
117. CR (3)Se 14	/166. LP*(8)Ag 10	5.11	10.73	0.214
153. LP (1)Se 7	/164. LP*(6)Ag 10	9.42	0.72	0.078
153. LP (1)Se 7	/165. LP*(7)Ag 10	4.10	0.84	0.053
153. LP (1)Se 7	/166. LP*(8)Ag 10	2.45	0.84	0.041
153. LP (1)Se 7	/167. LP*(9)Ag 10	10.34	0.82	0.082
154. LP (2)Se 7	/164. LP*(6)Ag 10	45.82	0.34	0.115
154. LP (2)Se 7	/165. LP*(7)Ag 10	3.77	0.46	0.038
154. LP (2)Se 7	/166. LP*(8)Ag 10	2.81	0.46	0.033
154. LP (2)Se 7	/167. LP*(9)Ag 10	9.93	0.45	0.061
154. LP (2)Se 7	/458. RY*(8)Ag 10	2.67	4.93	0.107
154. LP (2)Se 7	/460. RY*(10)Ag 10	1.40	2.55	0.056
154. LP (2)Se 7	/463. RY*(13)Ag 10	1.19	2.67	0.053
154. LP (2)Se 7	/467. RY*(17)Ag 10	4.43	37.40	0.379
154. LP (2)Se 7	/473. RY*(23)Ag 10	1.17	2.37	0.049
155. LP (1)Se 8	/164. LP*(6)Ag 10	7.14	0.76	0.070
155. LP (1)Se 8	/165. LP*(7)Ag 10	9.66	0.88	0.083
155. LP (1)Se 8	/167. LP*(9)Ag 10	4.41	0.86	0.055
156. LP (2)Se 8	/164. LP*(6)Ag 10	22.35	0.29	0.074
156. LP (2)Se 8	/165. LP*(7)Ag 10	7.29	0.41	0.049
156. LP (2)Se 8	/167. LP*(9)Ag 10	3.81	0.39	0.035
156. LP (2)Se 8	/458. RY*(8)Ag 10	1.06	4.87	0.067
156. LP (2)Se 8	/467. RY*(17)Ag 10	1.32	37.34	0.206
157. LP (1)Se 9	/164. LP*(6)Ag 10	2.37	0.77	0.041
157. LP (1)Se 9	/165. LP*(7)Ag 10	4.89	0.89	0.060
168. LP (1)Se 11	/164. LP*(6)Ag 10	1.53	0.76	0.032
168. LP (1)Se 11	/166. LP*(8)Ag 10	2.79	0.88	0.045
181. LP (1)Se 14	/164. LP*(6)Ag 10	5.15	0.77	0.060
181. LP (1)Se 14	/166. LP*(8)Ag 10	9.42	0.89	0.083
181. LP (1)Se 14	/167. LP*(9)Ag 10	1.48	0.88	0.032
182. LP (2)Se 14	/164. LP*(6)Ag 10	11.47	0.26	0.050
182. LP (2)Se 14	/166. LP*(8)Ag 10	5.43	0.37	0.041
9. BD (1)Se 7 -Se 9	/177. LP*(6)Ag 13	1.04	0.50	0.022
9. BD (1)Se 7 -Se 9	/179. LP*(8)Ag 13	2.32	0.62	0.034
10. BD (1)Se 7 -Se 11	/177. LP*(6)Ag 13	1.23	0.50	0.024
10. BD (1)Se 7 -Se 11	/178. LP*(7)Ag 13	2.09	0.62	0.033
10. BD (1)Se 7 -Se 11	/180. LP*(9)Ag 13	1.01	0.60	0.022
11. BD (1)Se 8 -Se 9	/177. LP*(6)Ag 13	1.44	0.50	0.026
11. BD (1)Se 8 -Se 9	/179. LP*(8)Ag 13	3.49	0.62	0.042
12. BD (1)Se 8 -Se 12	/177. LP*(6)Ag 13	2.26	0.50	0.032
12. BD (1)Se 8 -Se 12	/178. LP*(7)Ag 13	1.26	0.62	0.025
12. BD (1)Se 8 -Se 12	/179. LP*(8)Ag 13	2.34	0.62	0.035
12. BD (1)Se 8 -Se 12	/180. LP*(9)Ag 13	1.46	0.60	0.027
13. BD (1)Se 11 -Se 14	/177. LP*(6)Ag 13	2.58	0.50	0.035
13. BD (1)Se 11 -Se 14	/178. LP*(7)Ag 13	4.73	0.62	0.050
14. BD (1)Se 12 -Se 14	/177. LP*(6)Ag 13	3.06	0.50	0.038
14. BD (1)Se 12 -Se 14	/178. LP*(7)Ag 13	3.39	0.62	0.042
14. BD (1)Se 12 -Se 14	/180. LP*(9)Ag 13	1.35	0.60	0.026
53. CR (3)Se 8	/179. LP*(8)Ag 13	1.80	10.78	0.127
67. CR (3)Se 9	/177. LP*(6)Ag 13	2.22	10.61	0.147
67. CR (3)Se 9	/179. LP*(8)Ag 13	5.09	10.73	0.213
85. CR (3)Se 11	/177. LP*(6)Ag 13	3.50	10.66	0.186
85. CR (3)Se 11	/178. LP*(7)Ag 13	5.85	10.78	0.230
85. CR (3)Se 11	/180. LP*(9)Ag 13	2.17	10.76	0.138
99. CR (3)Se 12	/177. LP*(6)Ag 13	5.89	10.72	0.241
99. CR (3)Se 12	/178. LP*(7)Ag 13	3.07	10.84	0.167
99. CR (3)Se 12	/179. LP*(8)Ag 13	2.09	10.83	0.137
99. CR (3)Se 12	/180. LP*(9)Ag 13	5.45	10.82	0.219
117. CR (3)Se 14	/177. LP*(6)Ag 13	1.26	10.61	0.111
117. CR (3)Se 14	/178. LP*(7)Ag 13	2.98	10.73	0.164
155. LP (1)Se 8	/177. LP*(6)Ag 13	1.53	0.76	0.032
155. LP (1)Se 8	/179. LP*(8)Ag 13	2.81	0.88	0.045
157. LP (1)Se 9	/177. LP*(6)Ag 13	5.16	0.77	0.060
157. LP (1)Se 9	/179. LP*(8)Ag 13	9.38	0.89	0.083
157. LP (1)Se 9	/180. LP*(9)Ag 13	1.53	0.88	0.033
158. LP (2)Se 9	/177. LP*(6)Ag 13	11.53	0.26	0.050
158. LP (2)Se 9	/179. LP*(8)Ag 13	5.42	0.37	0.041
168. LP (1)Se 11	/177. LP*(6)Ag 13	7.07	0.76	0.070
168. LP (1)Se 11	/178. LP*(7)Ag 13	9.65	0.88	0.083
168. LP (1)Se 11	/180. LP*(9)Ag 13	4.30	0.86	0.054
169. LP (2)Se 11	/177. LP*(6)Ag 13	21.90	0.28	0.073
169. LP (2)Se 11	/178. LP*(7)Ag 13	7.21	0.40	0.049
169. LP (2)Se 11	/180. LP*(9)Ag 13	3.68	0.39	0.035
169. LP (2)Se 11	/561. RY*(8)Ag 13	1.04	4.88	0.066
169. LP (2)Se 11	/570. RY*(17)Ag 13	1.28	37.26	0.202

170.	LP (	1)Se	12		/177.	LP*(	6)Ag	13		9.43	0.72	0.078
170.	LP (	1)Se	12		/178.	LP*(	7)Ag	13		4.04	0.84	0.053
170.	LP (	1)Se	12		/179.	LP*(	8)Ag	13		2.48	0.84	0.041
170.	LP (	1)Se	12		/180.	LP*(	9)Ag	13		10.36	0.82	0.082
171.	LP (	2)Se	12		/177.	LP*(	6)Ag	13		46.05	0.34	0.116
171.	LP (	2)Se	12		/178.	LP*(	7)Ag	13		3.72	0.46	0.038
171.	LP (	2)Se	12		/179.	LP*(	8)Ag	13		2.84	0.46	0.033
171.	LP (	2)Se	12		/180.	LP*(	9)Ag	13		10.00	0.45	0.062
171.	LP (	2)Se	12		/561.	RY*(	8)Ag	13		2.70	4.94	0.108
171.	LP (	2)Se	12		/563.	RY*(	10)Ag	13		1.35	2.51	0.054
171.	LP (	2)Se	12		/566.	RY*(	13)Ag	13		1.18	2.65	0.052
171.	LP (	2)Se	12		/570.	RY*(	17)Ag	13		4.49	37.32	0.381
171.	LP (	2)Se	12		/576.	RY*(	23)Ag	13		1.17	2.37	0.049
181.	LP (	1)Se	14		/177.	LP*(	6)Ag	13		2.36	0.77	0.041
181.	LP (	1)Se	14		/178.	LP*(	7)Ag	13		4.84	0.89	0.060
164.	LP*(	6)Ag	10		/364.	RY*(	4)Se	7		1.12	0.53	0.058
164.	LP*(	6)Ag	10		/365.	RY*(	5)Se	7		1.05	0.55	0.057
164.	LP*(	6)Ag	10		/368.	RY*(	8)Se	7		2.15	0.88	0.105
164.	LP*(	6)Ag	10		/165.	LP*(	7)Ag	10		1.22	0.12	0.025
164.	LP*(	6)Ag	10		/456.	RY*(	6)Ag	10		1.43	1.44	0.109
164.	LP*(	6)Ag	10		/458.	RY*(	8)Ag	10		4.48	4.59	0.345
164.	LP*(	6)Ag	10		/460.	RY*(	10)Ag	10		2.06	2.21	0.162
164.	LP*(	6)Ag	10		/462.	RY*(	12)Ag	10		1.09	1.48	0.096
164.	LP*(	6)Ag	10		/463.	RY*(	13)Ag	10		1.92	2.32	0.161
164.	LP*(	6)Ag	10		/467.	RY*(	17)Ag	10		5.45	37.06	1.081
164.	LP*(	6)Ag	10		/471.	RY*(	21)Ag	10		1.00	1.85	0.104
164.	LP*(	6)Ag	10		/473.	RY*(	23)Ag	10		1.90	2.03	0.150
164.	LP*(	6)Ag	10		/178.	LP*(	7)Ag	13		1.84	0.12	0.031
164.	LP*(	6)Ag	10		/179.	LP*(	8)Ag	13		1.66	0.12	0.029
177.	LP*(	6)Ag	13		/527.	RY*(	4)Se	12		1.12	0.53	0.058
177.	LP*(	6)Ag	13		/528.	RY*(	5)Se	12		1.06	0.55	0.058
177.	LP*(	6)Ag	13		/531.	RY*(	8)Se	12		2.17	0.88	0.105
177.	LP*(	6)Ag	13		/165.	LP*(	7)Ag	10		1.86	0.12	0.031
177.	LP*(	6)Ag	13		/166.	LP*(	8)Ag	10		1.66	0.12	0.029
177.	LP*(	6)Ag	13		/178.	LP*(	7)Ag	13		1.18	0.12	0.025
177.	LP*(	6)Ag	13		/559.	RY*(	6)Ag	13		1.45	1.45	0.110
177.	LP*(	6)Ag	13		/561.	RY*(	8)Ag	13		4.48	4.59	0.346
177.	LP*(	6)Ag	13		/563.	RY*(	10)Ag	13		1.97	2.17	0.158
177.	LP*(	6)Ag	13		/565.	RY*(	12)Ag	13		1.18	1.50	0.101
177.	LP*(	6)Ag	13		/566.	RY*(	13)Ag	13		1.89	2.31	0.159
177.	LP*(	6)Ag	13		/570.	RY*(	17)Ag	13		5.46	36.98	1.082
177.	LP*(	6)Ag	13		/574.	RY*(	21)Ag	13		1.02	1.86	0.105
177.	LP*(	6)Ag	13		/576.	RY*(	23)Ag	13		1.88	2.02	0.148
15.	BD (	1) O	15 - S	17	/178.	LP*(	7)Ag	13		2.88	0.89	0.046
16.	BD (	2) O	15 - S	17	/178.	LP*(	7)Ag	13		1.15	0.60	0.024
20.	BD (	2) S	17 - O	19	/178.	LP*(	7)Ag	13		1.27	1.07	0.034
129.	CR (	1) O	15		/178.	LP*(	7)Ag	13		2.24	19.14	0.190
132.	CR (	2) S	17		/178.	LP*(	7)Ag	13		4.18	9.39	0.181
183.	LP (	1) O	15		/177.	LP*(	6)Ag	13		6.00	0.82	0.066
183.	LP (	1) O	15		/178.	LP*(	7)Ag	13		12.69	0.94	0.099
183.	LP (	1) O	15		/179.	LP*(	8)Ag	13		1.64	0.93	0.035
183.	LP (	1) O	15		/180.	LP*(	9)Ag	13		1.36	0.92	0.032
184.	LP (	2) O	15		/177.	LP*(	6)Ag	13		5.26	0.33	0.039
184.	LP (	2) O	15		/178.	LP*(	7)Ag	13		2.77	0.45	0.032
187.	LP (	1) S	17		/177.	LP*(	6)Ag	13		1.01	0.61	0.024
187.	LP (	1) S	17		/178.	LP*(	7)Ag	13		9.33	0.73	0.075
189.	LP (	1) O	19		/178.	LP*(	7)Ag	13		2.76	0.93	0.046
15.	BD (	1) O	15 - S	17	/744.	RY*(	2) O	19		1.25	1.95	0.045
15.	BD (	1) O	15 - S	17	/760.	RY*(	18) O	19		1.14	2.28	0.046
15.	BD (	1) O	15 - S	17	/810.	BD*(	2) O	15 - S	17	22.37	1.09	0.143
15.	BD (	1) O	15 - S	17	/813.	BD*(	1) S	17 - O	19	20.43	1.07	0.135
16.	BD (	2) O	15 - S	17	/744.	RY*(	2) O	19		2.59	1.67	0.060
16.	BD (	2) O	15 - S	17	/760.	RY*(	18) O	19		2.44	2.00	0.064
16.	BD (	2) O	15 - S	17	/809.	BD*(	1) O	15 - S	17	19.49	0.83	0.114
16.	BD (	2) O	15 - S	17	/810.	BD*(	2) O	15 - S	17	2.08	0.81	0.037
16.	BD (	2) O	15 - S	17	/813.	BD*(	1) S	17 - O	19	47.38	0.78	0.173
16.	BD (	2) O	15 - S	17	/814.	BD*(	2) S	17 - O	19	1.90	0.88	0.037
19.	BD (	1) S	17 - O	19	/629.	RY*(	3) O	15		2.52	1.20	0.051
19.	BD (	1) S	17 - O	19	/633.	RY*(	7) O	15		1.74	2.14	0.057
19.	BD (	1) S	17 - O	19	/744.	RY*(	2) O	19		1.48	1.52	0.044
19.	BD (	1) S	17 - O	19	/760.	RY*(	18) O	19		1.32	1.85	0.046
19.	BD (	1) S	17 - O	19	/809.	BD*(	1) O	15 - S	17	20.52	0.68	0.106
19.	BD (	1) S	17 - O	19	/810.	BD*(	2) O	15 - S	17	60.61	0.66	0.179
19.	BD (	1) S	17 - O	19	/813.	BD*(	1) S	17 - O	19	16.34	0.63	0.091
19.	BD (	1) S	17 - O	19	/814.	BD*(	2) S	17 - O	19	1.20	0.73	0.027
20.	BD (	2) S	17 - O	19	/810.	BD*(	2) O	15 - S	17	3.15	1.27	0.059
20.	BD (	2) S	17 - O	19	/813.	BD*(	1) S	17 - O	19	1.33	1.25	0.038
141.	CR (	1) O	19		/680.	RY*(	2) S	17		1.25	19.92	0.142
141.	CR (	1) O	19		/681.	RY*(	3) S	17		1.01	20.65	0.129
183.	LP (	1) O	15		/682.	RY*(	4) S	17		3.20	2.36	0.079
183.	LP (	1) O	15		/814.	BD*(	2) S	17 - O	19	1.53	1.21	0.039
184.	LP (	2) O	15		/679.	RY*(	1) S	17		11.32	1.03	0.098

184. LP (2) O 15	/680. RY*(2) S 17	3.47	1.27	0.061
184. LP (2) O 15	/814. BD*(2) S 17 - O 19	17.64	0.73	0.103
189. LP (1) O 19	/681. RY*(3) S 17	4.26	2.47	0.092
190. LP (2) O 19	/679. RY*(1) S 17	20.36	0.99	0.130
190. LP (2) O 19	/809. BD*(1) O 15 - S 17	19.51	0.64	0.101
190. LP (2) O 19	/810. BD*(2) O 15 - S 17	7.84	0.62	0.062
809. BD*(1) O 15 - S 17	/630. RY*(4) O 15	1.03	1.10	0.116
809. BD*(1) O 15 - S 17	/679. RY*(1) S 17	10.21	0.36	0.167
809. BD*(1) O 15 - S 17	/680. RY*(2) S 17	9.02	0.59	0.226
809. BD*(1) O 15 - S 17	/814. BD*(2) S 17 - O 19	1.53	0.06	0.025
810. BD*(2) O 15 - S 17	/629. RY*(3) O 15	1.78	0.54	0.096
810. BD*(2) O 15 - S 17	/633. RY*(7) O 15	1.27	1.48	0.135
810. BD*(2) O 15 - S 17	/679. RY*(1) S 17	4.10	0.38	0.102
810. BD*(2) O 15 - S 17	/680. RY*(2) S 17	3.64	0.62	0.134
810. BD*(2) O 15 - S 17	/684. RY*(6) S 17	1.06	0.77	0.089
810. BD*(2) O 15 - S 17	/744. RY*(2) O 19	1.77	0.86	0.121
810. BD*(2) O 15 - S 17	/760. RY*(18) O 19	1.40	1.19	0.127
810. BD*(2) O 15 - S 17	/809. BD*(1) O 15 - S 17	1.60	0.02	0.013
810. BD*(2) O 15 - S 17	/814. BD*(2) S 17 - O 19	8.75	0.08	0.065
813. BD*(1) S 17 - O 19	/629. RY*(3) O 15	1.34	0.56	0.094
813. BD*(1) S 17 - O 19	/704. RY*(26) S 17	1.07	2.00	0.158
813. BD*(1) S 17 - O 19	/744. RY*(2) O 19	1.77	0.88	0.135
813. BD*(1) S 17 - O 19	/760. RY*(18) O 19	3.39	1.21	0.219
813. BD*(1) S 17 - O 19	/809. BD*(1) O 15 - S 17	127.29	0.04	0.181
813. BD*(1) S 17 - O 19	/810. BD*(2) O 15 - S 17	745.75	0.02	0.303
17. BD (1) O 16 - S 18	/179. LP*(8)Ag 13	3.35	0.83	0.047
18. BD (2) O 16 - S 18	/179. LP*(8)Ag 13	1.79	0.66	0.031
130. CR (1) O 16	/179. LP*(8)Ag 13	2.27	19.13	0.190
137. CR (2) S 18	/179. LP*(8)Ag 13	3.13	9.38	0.156
185. LP (1) O 16	/177. LP*(6)Ag 13	4.55	0.82	0.058
185. LP (1) O 16	/179. LP*(8)Ag 13	14.86	0.93	0.106
186. LP (2) O 16	/177. LP*(6)Ag 13	3.04	0.32	0.029
186. LP (2) O 16	/179. LP*(8)Ag 13	1.75	0.44	0.025
188. LP (1) S 18	/177. LP*(6)Ag 13	1.16	0.61	0.025
188. LP (1) S 18	/179. LP*(8)Ag 13	7.01	0.73	0.065
191. LP (1) O 20	/178. LP*(7)Ag 13	1.04	0.93	0.028
191. LP (1) O 20	/179. LP*(8)Ag 13	1.30	0.93	0.032
17. BD (1) O 16 - S 18	/771. RY*(3) O 20	1.00	1.85	0.039
17. BD (1) O 16 - S 18	/812. BD*(2) O 16 - S 18	24.46	1.04	0.145
17. BD (1) O 16 - S 18	/815. BD*(1) S 18 - O 20	27.70	1.01	0.152
18. BD (2) O 16 - S 18	/771. RY*(3) O 20	2.49	1.68	0.059
18. BD (2) O 16 - S 18	/811. BD*(1) O 16 - S 18	22.91	0.88	0.128
18. BD (2) O 16 - S 18	/812. BD*(2) O 16 - S 18	1.00	0.87	0.026
18. BD (2) O 16 - S 18	/815. BD*(1) S 18 - O 20	40.50	0.84	0.166
18. BD (2) O 16 - S 18	/816. BD*(2) S 18 - O 20	3.53	0.92	0.051
21. BD (1) S 18 - O 20	/655. RY*(3) O 16	2.65	1.31	0.055
21. BD (1) S 18 - O 20	/659. RY*(7) O 16	1.02	2.37	0.046
21. BD (1) S 18 - O 20	/660. RY*(8) O 16	1.12	2.26	0.047
21. BD (1) S 18 - O 20	/666. RY*(14) O 16	1.21	2.11	0.047
21. BD (1) S 18 - O 20	/739. RY*(29) S 18	1.24	2.64	0.053
21. BD (1) S 18 - O 20	/771. RY*(3) O 20	1.29	1.49	0.041
21. BD (1) S 18 - O 20	/811. BD*(1) O 16 - S 18	27.56	0.69	0.124
21. BD (1) S 18 - O 20	/812. BD*(2) O 16 - S 18	45.46	0.68	0.157
21. BD (1) S 18 - O 20	/815. BD*(1) S 18 - O 20	13.51	0.65	0.084
21. BD (1) S 18 - O 20	/816. BD*(2) S 18 - O 20	2.90	0.73	0.042
22. BD (2) S 18 - O 20	/812. BD*(2) O 16 - S 18	5.04	1.26	0.074
22. BD (2) S 18 - O 20	/815. BD*(1) S 18 - O 20	3.27	1.23	0.059
142. CR (1) O 20	/712. RY*(2) S 18	1.17	19.93	0.138
185. LP (1) O 16	/714. RY*(4) S 18	3.34	2.36	0.080
185. LP (1) O 16	/816. BD*(2) S 18 - O 20	1.08	1.20	0.033
186. LP (2) O 16	/711. RY*(1) S 18	13.21	1.00	0.105
186. LP (2) O 16	/712. RY*(2) S 18	3.03	1.26	0.057
186. LP (2) O 16	/815. BD*(1) S 18 - O 20	1.00	0.62	0.022
186. LP (2) O 16	/816. BD*(2) S 18 - O 20	19.20	0.70	0.105
191. LP (1) O 20	/713. RY*(3) S 18	4.39	2.59	0.095
192. LP (2) O 20	/711. RY*(1) S 18	18.91	0.99	0.125
192. LP (2) O 20	/712. RY*(2) S 18	1.28	1.24	0.037
192. LP (2) O 20	/811. BD*(1) O 16 - S 18	16.55	0.64	0.093
192. LP (2) O 20	/812. BD*(2) O 16 - S 18	10.06	0.63	0.071
811. BD*(1) O 16 - S 18	/711. RY*(1) S 18	7.47	0.34	0.140
811. BD*(1) O 16 - S 18	/712. RY*(2) S 18	9.02	0.60	0.225
812. BD*(2) O 16 - S 18	/655. RY*(3) O 16	1.35	0.63	0.094
812. BD*(2) O 16 - S 18	/666. RY*(14) O 16	1.07	1.43	0.126
812. BD*(2) O 16 - S 18	/711. RY*(1) S 18	4.49	0.36	0.107
812. BD*(2) O 16 - S 18	/712. RY*(2) S 18	5.40	0.61	0.168
812. BD*(2) O 16 - S 18	/716. RY*(6) S 18	2.06	0.31	0.081
812. BD*(2) O 16 - S 18	/739. RY*(29) S 18	1.17	1.96	0.155
812. BD*(2) O 16 - S 18	/771. RY*(3) O 20	1.26	0.82	0.103
812. BD*(2) O 16 - S 18	/811. BD*(1) O 16 - S 18	4.93	0.02	0.021
812. BD*(2) O 16 - S 18	/816. BD*(2) S 18 - O 20	19.73	0.06	0.085
815. BD*(1) S 18 - O 20	/655. RY*(3) O 16	1.49	0.65	0.104
815. BD*(1) S 18 - O 20	/716. RY*(6) S 18	1.82	0.33	0.082

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 815. BD*(   1) S  18 - O  20        /739. RY*(  29) S  18                    1.12    1.99    0.157
 815. BD*(   1) S  18 - O  20        /771. RY*(   3) O  20                    1.40    0.84    0.114
 815. BD*(   1) S  18 - O  20        /811. BD*(   1) O  16 - S  18          192.20    0.04    0.213
 815. BD*(   1) S  18 - O  20        /812. BD*(   2) O  16 - S  18          545.80    0.03    0.272

 Wiberg bond index matrix in the NAO basis:

     Atom    1       2       3       4       5       6       7       8       9
     ---- ------  ------  ------  ------  ------  ------  ------  ------  ------
   1.  S  0.0000  0.0004  1.3929  1.6238  0.0010  0.0002  0.0010  0.0007  0.0004
   2.  S  0.0004  0.0000  0.0008  0.0002  1.4421  1.5780  0.0016  0.0021  0.0008
   3.  O  1.3929  0.0008  0.0000  0.2599  0.0016  0.0002  0.0032  0.0017  0.0007
   4.  O  1.6238  0.0002  0.2599  0.0000  0.0003  0.0001  0.0006  0.0003  0.0002
   5.  O  0.0010  1.4421  0.0016  0.0003  0.0000  0.2608  0.0021  0.0022  0.0009
   6.  O  0.0002  1.5780  0.0002  0.0001  0.2608  0.0000  0.0007  0.0064  0.0008
   7. Se  0.0010  0.0016  0.0032  0.0006  0.0021  0.0007  0.0000  0.0788  0.9967
   8. Se  0.0007  0.0021  0.0017  0.0003  0.0022  0.0064  0.0788  0.0000  1.0253
   9. Se  0.0004  0.0008  0.0007  0.0002  0.0009  0.0008  0.9967  1.0253  0.0000
  10. Ag  0.0623  0.0487  0.1236  0.0357  0.1018  0.0270  0.2429  0.1589  0.0306
  11. Se  0.0002  0.0003  0.0004  0.0002  0.0007  0.0002  0.9753  0.0142  0.0875
  12. Se  0.0001  0.0012  0.0003  0.0001  0.0009  0.0046  0.0143  0.9747  0.0819
  13. Ag  0.0001  0.0001  0.0002  0.0000  0.0002  0.0001  0.0162  0.0255  0.1179
  14. Se  0.0009  0.0006  0.0015  0.0005  0.0016  0.0004  0.0819  0.0875  0.0148
  15.  O  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0003  0.0004  0.0015
  16.  O  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0009  0.0007  0.0016
  17.  S  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0001  0.0002  0.0009
  18.  S  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0012  0.0003  0.0006
  19.  O  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0001  0.0002  0.0005
  20.  O  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0046  0.0002  0.0004

     Atom   10      11      12      13      14      15      16      17      18
     ---- ------  ------  ------  ------  ------  ------  ------  ------  ------
   1.  S  0.0623  0.0002  0.0001  0.0001  0.0009  0.0000  0.0000  0.0000  0.0000
   2.  S  0.0487  0.0003  0.0012  0.0001  0.0006  0.0000  0.0000  0.0000  0.0000
   3.  O  0.1236  0.0004  0.0003  0.0002  0.0015  0.0000  0.0000  0.0000  0.0000
   4.  O  0.0357  0.0002  0.0001  0.0000  0.0005  0.0000  0.0000  0.0000  0.0000
   5.  O  0.1018  0.0007  0.0009  0.0002  0.0016  0.0000  0.0000  0.0000  0.0000
   6.  O  0.0270  0.0002  0.0046  0.0001  0.0004  0.0000  0.0000  0.0000  0.0000
   7. Se  0.2429  0.9753  0.0143  0.0162  0.0819  0.0003  0.0009  0.0001  0.0012
   8. Se  0.1589  0.0142  0.9747  0.0255  0.0875  0.0004  0.0007  0.0002  0.0003
   9. Se  0.0306  0.0875  0.0819  0.1179  0.0148  0.0015  0.0016  0.0009  0.0006
  10. Ag  0.0000  0.0255  0.0163  0.0164  0.1177  0.0002  0.0002  0.0001  0.0001
  11. Se  0.0255  0.0000  0.0789  0.1573  1.0257  0.0017  0.0022  0.0007  0.0021
  12. Se  0.0163  0.0789  0.0000  0.2435  0.9965  0.0032  0.0021  0.0010  0.0016
  13. Ag  0.0164  0.1573  0.2435  0.0000  0.0306  0.1235  0.1019  0.0621  0.0487
  14. Se  0.1177  1.0257  0.9965  0.0306  0.0000  0.0007  0.0009  0.0004  0.0008
  15.  O  0.0002  0.0017  0.0032  0.1235  0.0007  0.0000  0.0016  1.3923  0.0008
  16.  O  0.0002  0.0022  0.0021  0.1019  0.0009  0.0016  0.0000  0.0010  1.4416
  17.  S  0.0001  0.0007  0.0010  0.0621  0.0004  1.3923  0.0010  0.0000  0.0004
  18.  S  0.0001  0.0021  0.0016  0.0487  0.0008  0.0008  1.4416  0.0004  0.0000
  19.  O  0.0000  0.0003  0.0006  0.0354  0.0002  0.2599  0.0003  1.6244  0.0002
  20.  O  0.0001  0.0065  0.0007  0.0269  0.0008  0.0002  0.2608  0.0002  1.5784

     Atom   19      20
     ---- ------  ------
   1.  S  0.0000  0.0000
   2.  S  0.0000  0.0000
   3.  O  0.0000  0.0000
   4.  O  0.0000  0.0000
   5.  O  0.0000  0.0000
   6.  O  0.0000  0.0000
   7. Se  0.0001  0.0046
   8. Se  0.0002  0.0002
   9. Se  0.0005  0.0004
  10. Ag  0.0000  0.0001
  11. Se  0.0003  0.0065
  12. Se  0.0006  0.0007
  13. Ag  0.0354  0.0269
  14. Se  0.0002  0.0008
  15.  O  0.2599  0.0002
  16.  O  0.0003  0.2608
  17.  S  1.6244  0.0002
  18.  S  0.0002  1.5784
  19.  O  0.0000  0.0001
  20.  O  0.0001  0.0000

Summary of Natural Population Analysis:
                                     Natural Population
                 Natural   -----------------------------------
Atom No          Charge        Core        Valence     Rydberg     Total
               -----------------------------------------------------------
  1  s            1.69542     9.99909     4.10197     0.20351    14.30458
```

2	s	1.69233	9.99912	4.10234	0.20621	14.30767
3	o	-0.89705	1.99985	6.86011	0.03709	8.89705
4	o	-0.74612	1.99986	6.70412	0.04214	8.74612
5	o	-0.87223	1.99985	6.83418	0.03820	8.87223
6	o	-0.77970	1.99985	6.73882	0.04103	8.77970
7	se	0.00768	27.99925	5.92985	0.06322	33.99232
8	se	0.06673	27.99926	5.87834	0.05566	33.93327
9	se	0.08248	27.99926	5.86761	0.05065	33.91752
10	ag	0.74998	7.99893	10.22510	0.02599	18.25002
11	se	0.06779	27.99926	5.87745	0.05551	33.93221
12	se	0.00720	27.99925	5.93021	0.06333	33.99280
13	ag	0.75058	7.99893	10.22454	0.02595	18.24942
14	se	0.08246	27.99926	5.86766	0.05062	33.91754
15	o	-0.89768	1.99985	6.86082	0.03701	8.89768
16	o	-0.87255	1.99985	6.83454	0.03816	8.87255
17	s	1.69537	9.99909	4.10198	0.20356	14.30463
18	s	1.69246	9.99912	4.10222	0.20620	14.30754
19	o	-0.74569	1.99986	6.70367	0.04216	8.74569
20	o	-0.77946	1.99985	6.73857	0.04104	8.77946
* Total *		2.00000	239.98864	126.48410	1.52725	368.00000

For all atoms:

Core	239.98864(	99.9953% of 240)
Valence	126.48410(	98.8157% of 128)
Natural Minimal Basis	366.47275(	99.5850% of 368)
Natural Rydberg Basis	1.52725(	0.4150% of 368)

atomic charges with multicenter corrections

atom	charge
1 s	1.1779
2 s	1.1824
3 o	-0.6120
4 o	-0.4676
5 o	-0.5912
6 o	-0.5122
7 se	0.1963
8 se	0.1144
9 se	0.0894
10 ag	0.4226
11 se	0.1134
12 se	0.1975
13 ag	0.4229
14 se	0.0890
15 o	-0.6127
16 o	-0.5916
17 s	1.1782
18 s	1.1825
19 o	-0.4672
20 o	-0.5120

$Ag_2Se_6^{2+}$ **(A)**

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 1.00 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
1. BD (1)Se 1 -Se 4	/ 3. BD*(2)Se 1 -Se 4	1.28	0.26	0.045
1. BD (1)Se 1 -Se 4	/115. LP*(6)Ag 7	1.72	0.64	0.030
1. BD (1)Se 1 -Se 4	/116. LP*(7)Ag 7	1.26	0.74	0.027
1. BD (1)Se 1 -Se 4	/122. LP (6)Ag 8	1.72	0.64	0.030
1. BD (1)Se 1 -Se 4	/123. LP*(7)Ag 8	1.26	0.74	0.027
2. BD (2)Se 1 -Se 4	/115. LP*(6)Ag 7	2.96	0.45	0.033
2. BD (2)Se 1 -Se 4	/122. LP (6)Ag 8	2.96	0.45	0.033
2. BD (2)Se 1 -Se 4	/315. RY*(11)Ag 7	1.03	41.22	0.187
2. BD (2)Se 1 -Se 4	/356. RY*(9)Ag 8	1.03	41.22	0.187
2. BD (2)Se 1 -Se 4	/394. BD*(1)Se 2 -Se 5	1.34	0.29	0.018

2. BD (2)Se 1 -Se 4	/395. BD*(1)Se 2 -Ag 7	2.18	0.44	0.028
2. BD (2)Se 1 -Se 4	/396. BD*(1)Se 3 -Se 6	1.34	0.29	0.018
2. BD (2)Se 1 -Se 4	/397. BD*(1)Se 3 -Ag 8	2.18	0.44	0.028
2. BD (2)Se 1 -Se 4	/399. BD*(1)Se 5 -Ag 8	1.59	0.44	0.024
2. BD (2)Se 1 -Se 4	/400. BD*(1)Se 6 -Ag 7	1.59	0.44	0.024
3. BD*(2)Se 1 -Se 4	/115. LP*(6)Ag 7	4.70	0.39	0.040
3. BD*(2)Se 1 -Se 4	/122. LP (6)Ag 8	4.70	0.39	0.040
3. BD*(2)Se 1 -Se 4	/125. RY*(1)Se 1	2.85	0.84	0.046
3. BD*(2)Se 1 -Se 4	/215. RY*(1)Se 4	2.85	0.84	0.046
3. BD*(2)Se 1 -Se 4	/315. RY*(11)Ag 7	1.00	41.16	0.193
3. BD*(2)Se 1 -Se 4	/356. RY*(9)Ag 8	1.00	41.16	0.193
3. BD*(2)Se 1 -Se 4	/392. BD*(1)Se 1 -Se 5	4.72	0.23	0.031
3. BD*(2)Se 1 -Se 4	/394. BD*(1)Se 2 -Se 5	2.51	0.23	0.022
3. BD*(2)Se 1 -Se 4	/395. BD*(1)Se 2 -Ag 7	2.95	0.38	0.031
3. BD*(2)Se 1 -Se 4	/396. BD*(1)Se 3 -Se 6	2.51	0.23	0.022
3. BD*(2)Se 1 -Se 4	/397. BD*(1)Se 3 -Ag 8	2.95	0.38	0.031
3. BD*(2)Se 1 -Se 4	/398. BD*(1)Se 4 -Se 6	4.72	0.23	0.031
3. BD*(2)Se 1 -Se 4	/399. BD*(1)Se 5 -Ag 8	4.38	0.38	0.038
3. BD*(2)Se 1 -Se 4	/400. BD*(1)Se 6 -Ag 7	4.38	0.38	0.038
4. BD (1)Se 1 -Se 5	/115. LP*(6)Ag 7	2.12	0.65	0.033
4. BD (1)Se 1 -Se 5	/116. LP*(7)Ag 7	1.30	0.74	0.028
4. BD (1)Se 1 -Se 5	/123. LP*(7)Ag 8	1.59	0.74	0.031
4. BD (1)Se 1 -Se 5	/399. BD*(1)Se 5 -Ag 8	1.53	0.64	0.028
5. BD (1)Se 2 -Se 3	/116. LP*(7)Ag 7	1.64	0.74	0.031
5. BD (1)Se 2 -Se 3	/123. LP*(7)Ag 8	1.64	0.74	0.031
5. BD (1)Se 2 -Se 3	/395. BD*(1)Se 2 -Ag 7	1.14	0.63	0.024
5. BD (1)Se 2 -Se 3	/397. BD*(1)Se 3 -Ag 8	1.14	0.63	0.024
6. BD (1)Se 2 -Se 5	/116. LP*(7)Ag 7	1.54	0.74	0.030
6. BD (1)Se 2 -Se 5	/123. LP*(7)Ag 8	1.64	0.74	0.031
6. BD (1)Se 2 -Se 5	/395. BD*(1)Se 2 -Ag 7	1.46	0.63	0.028
6. BD (1)Se 2 -Se 5	/399. BD*(1)Se 5 -Ag 8	1.14	0.63	0.024
7. BD (1)Se 2 -Ag 7	/392. BD*(1)Se 1 -Se 5	2.82	0.28	0.025
7. BD (1)Se 2 -Ag 7	/396. BD*(1)Se 3 -Se 6	2.95	0.29	0.026
7. BD (1)Se 2 -Ag 7	/400. BD*(1)Se 6 -Ag 7	4.29	0.43	0.039
8. BD (1)Se 3 -Se 6	/116. LP*(7)Ag 7	1.64	0.74	0.031
8. BD (1)Se 3 -Se 6	/123. LP*(7)Ag 8	1.54	0.74	0.030
8. BD (1)Se 3 -Se 6	/397. BD*(1)Se 3 -Ag 8	1.46	0.63	0.028
8. BD (1)Se 3 -Se 6	/400. BD*(1)Se 6 -Ag 7	1.14	0.63	0.024
9. BD (1)Se 3 -Ag 8	/394. BD*(1)Se 2 -Se 5	2.95	0.29	0.026
9. BD (1)Se 3 -Ag 8	/398. BD*(1)Se 4 -Se 6	2.82	0.28	0.025
9. BD (1)Se 3 -Ag 8	/399. BD*(1)Se 5 -Ag 8	4.29	0.43	0.039
10. BD (1)Se 4 -Se 6	/116. LP*(7)Ag 7	1.59	0.74	0.031
10. BD (1)Se 4 -Se 6	/122. LP (6)Ag 8	2.12	0.65	0.033
10. BD (1)Se 4 -Se 6	/123. LP*(7)Ag 8	1.30	0.74	0.028
10. BD (1)Se 4 -Se 6	/400. BD*(1)Se 6 -Ag 7	1.53	0.64	0.028
11. BD (1)Se 5 -Ag 8	/391. BD*(1)Se 1 -Se 4	3.10	0.29	0.027
11. BD (1)Se 5 -Ag 8	/393. BD*(1)Se 2 -Se 3	2.95	0.29	0.026
11. BD (1)Se 5 -Ag 8	/397. BD*(1)Se 3 -Ag 8	4.29	0.43	0.039
12. BD (1)Se 6 -Ag 7	/391. BD*(1)Se 1 -Se 4	3.10	0.29	0.027
12. BD (1)Se 6 -Ag 7	/393. BD*(1)Se 2 -Se 3	2.95	0.29	0.026
12. BD (1)Se 6 -Ag 7	/395. BD*(1)Se 2 -Ag 7	4.29	0.43	0.039
15. CR (3)Se 1	/115. LP*(6)Ag 7	4.63	10.79	0.201
15. CR (3)Se 1	/116. LP*(7)Ag 7	1.59	10.89	0.118
15. CR (3)Se 1	/123. LP*(7)Ag 8	1.01	10.89	0.094
29. CR (3)Se 2	/116. LP*(7)Ag 7	2.29	10.89	0.141
29. CR (3)Se 2	/123. LP*(7)Ag 8	1.25	10.89	0.104
29. CR (3)Se 2	/395. BD*(1)Se 2 -Ag 7	2.97	10.78	0.163
43. CR (3)Se 3	/116. LP*(7)Ag 7	1.25	10.89	0.104
43. CR (3)Se 3	/123. LP*(7)Ag 8	2.29	10.89	0.141
43. CR (3)Se 3	/397. BD*(1)Se 3 -Ag 8	2.97	10.78	0.163
57. CR (3)Se 4	/116. LP*(7)Ag 7	1.01	10.89	0.094
57. CR (3)Se 4	/122. LP (6)Ag 8	4.63	10.79	0.201
57. CR (3)Se 4	/123. LP*(7)Ag 8	1.59	10.89	0.118
71. CR (3)Se 5	/116. LP*(7)Ag 7	1.01	10.89	0.094
71. CR (3)Se 5	/123. LP*(7)Ag 8	2.29	10.89	0.141
71. CR (3)Se 5	/399. BD*(1)Se 5 -Ag 8	2.97	10.78	0.163
85. CR (3)Se 6	/116. LP*(7)Ag 7	2.29	10.89	0.141
85. CR (3)Se 6	/123. LP*(7)Ag 8	1.01	10.89	0.094
85. CR (3)Se 6	/400. BD*(1)Se 6 -Ag 7	2.97	10.78	0.163
105. LP (1)Se 1	/ 3. BD*(2)Se 1 -Se 4	1.00	0.52	0.055
105. LP (1)Se 1	/115. LP*(6)Ag 7	8.31	0.91	0.078
105. LP (1)Se 1	/116. LP*(7)Ag 7	1.94	1.01	0.040
105. LP (1)Se 1	/123. LP*(7)Ag 8	1.29	1.01	0.032
105. LP (1)Se 1	/395. BD*(1)Se 2 -Ag 7	1.89	0.90	0.037
105. LP (1)Se 1	/399. BD*(1)Se 5 -Ag 8	1.63	0.90	0.035
105. LP (1)Se 1	/400. BD*(1)Se 6 -Ag 7	1.89	0.90	0.037
106. LP (1)Se 2	/116. LP*(7)Ag 7	2.94	1.00	0.049
106. LP (1)Se 2	/123. LP*(7)Ag 8	1.60	1.00	0.036
106. LP (1)Se 2	/395. BD*(1)Se 2 -Ag 7	5.51	0.90	0.064
107. LP (1)Se 3	/116. LP*(7)Ag 7	1.60	1.00	0.036
107. LP (1)Se 3	/123. LP*(7)Ag 8	2.94	1.00	0.049
107. LP (1)Se 3	/397. BD*(1)Se 3 -Ag 8	5.51	0.90	0.064

108. LP (1)Se 4	/ 3. BD*(2)Se 1 -Se 4	1.00	0.52	0.055
108. LP (1)Se 4	/116. LP*(7)Ag 7	1.29	1.01	0.032
108. LP (1)Se 4	/122. LP (6)Ag 8	8.31	0.91	0.078
108. LP (1)Se 4	/123. LP*(7)Ag 8	1.94	1.01	0.040
108. LP (1)Se 4	/397. BD*(1)Se 3 -Ag 8	1.89	0.90	0.037
108. LP (1)Se 4	/399. BD*(1)Se 5 -Ag 8	1.89	0.90	0.037
108. LP (1)Se 4	/400. BD*(1)Se 6 -Ag 7	1.63	0.90	0.035
109. LP (1)Se 5	/116. LP*(7)Ag 7	1.29	1.00	0.032
109. LP (1)Se 5	/123. LP*(7)Ag 8	2.94	1.00	0.049
109. LP (1)Se 5	/395. BD*(1)Se 2 -Ag 7	1.62	0.90	0.034
109. LP (1)Se 5	/399. BD*(1)Se 5 -Ag 8	5.51	0.90	0.064
110. LP (1)Se 6	/116. LP*(7)Ag 7	2.94	1.00	0.049
110. LP (1)Se 6	/123. LP*(7)Ag 8	1.29	1.00	0.032
110. LP (1)Se 6	/397. BD*(1)Se 3 -Ag 8	1.62	0.90	0.034
110. LP (1)Se 6	/400. BD*(1)Se 6 -Ag 7	5.51	0.90	0.064

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8
1. Se	0.0000	0.0794	0.0132	1.0037	1.0037	0.0794	0.1661	0.0211
2. Se	0.0794	0.0000	1.0037	0.0132	1.0037	0.0794	0.1661	0.0211
3. Se	0.0132	1.0037	0.0000	0.0794	0.0794	1.0037	0.0211	0.1661
4. Se	1.0037	0.0132	0.0794	0.0000	0.0794	1.0037	0.0211	0.1661
5. Se	1.0037	1.0037	0.0794	0.0794	0.0000	0.0132	0.0211	0.1661
6. Se	0.0794	0.0794	1.0037	1.0037	0.0132	0.0000	0.1661	0.0211
7. Ag	0.1661	0.1661	0.0211	0.0211	0.0211	0.1661	0.0000	0.0180
8. Ag	0.0211	0.0211	0.1661	0.1661	0.1661	0.0211	0.0180	0.0000

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
1 se	0.07063	27.99931	5.86922	0.06084	33.92937
2 se	0.07063	27.99931	5.86922	0.06084	33.92937
3 se	0.07063	27.99931	5.86922	0.06084	33.92937
4 se	0.07063	27.99931	5.86922	0.06084	33.92937
5 se	0.07063	27.99931	5.86922	0.06084	33.92937
6 se	0.07063	27.99931	5.86922	0.06084	33.92937
7 ag	0.78812	7.99937	10.19313	0.01939	18.21188
8 ag	0.78812	7.99937	10.19313	0.01939	18.21188
* Total *	2.00000	183.99461	55.60158	0.40381	240.00000

For all atoms:

Core	183.99461(	99.9971% of	184)
Valence	55.60158(	99.2885% of	56)
Natural Minimal Basis	239.59619(	99.8317% of	240)
Natural Rydberg Basis	0.40381(	0.1683% of	240)

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**********************************************************************
*                                                                    *
*              atomic charges with multicenter corrections           *
*                                                                    *
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atom	charge
1 se	0.1930
2 se	0.1930
3 se	0.1930
4 se	0.1930
5 se	0.1930
6 se	0.1930
7 ag	0.4209
8 ag	0.4209

$Ag_3(Se_6)_2^{3+}$ **(C)**

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 1.00 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.

3. BD (1)Se 1 -Ag 13	/394. RY*(3)Se 6	2.05	1.28	0.047
3. BD (1)Se 1 -Ag 13	/397. RY*(6)Se 6	1.04	0.99	0.029
3. BD (1)Se 1 -Ag 13	/613. RY*(12)Ag 13	1.56	4.19	0.074
3. BD (1)Se 1 -Ag 13	/614. RY*(13)Ag 13	2.07	42.37	0.271
3. BD (1)Se 1 -Ag 13	/737. BD*(1)Se 3 -Se 9	2.97	0.40	0.031
3. BD (1)Se 1 -Ag 13	/742. BD*(1)Se 6 -Ag 13	15.14	0.51	0.079
3. BD (1)Se 1 -Ag 13	/743. BD*(1)Se 7 -Se 11	2.97	0.40	0.031
12. BD (1)Se 6 -Ag 13	/244. RY*(3)Se 1	2.05	1.28	0.047
12. BD (1)Se 6 -Ag 13	/247. RY*(6)Se 1	1.04	0.99	0.029
12. BD (1)Se 6 -Ag 13	/613. RY*(12)Ag 13	1.56	4.19	0.074
12. BD (1)Se 6 -Ag 13	/614. RY*(13)Ag 13	2.07	42.37	0.271
12. BD (1)Se 6 -Ag 13	/733. BD*(1)Se 1 -Ag 13	15.14	0.51	0.079
12. BD (1)Se 6 -Ag 13	/739. BD*(1)Se 4 -Se 10	2.97	0.40	0.031
12. BD (1)Se 6 -Ag 13	/744. BD*(1)Se 8 -Se 12	2.97	0.40	0.031
17. CR (3)Se 1	/222. LP*(6)Ag 13	1.19	10.88	0.102
17. CR (3)Se 1	/733. BD*(1)Se 1 -Ag 13	1.81	10.80	0.127
87. CR (3)Se 6	/222. LP*(6)Ag 13	1.19	10.88	0.102
87. CR (3)Se 6	/742. BD*(1)Se 6 -Ag 13	1.81	10.80	0.127
195. LP (1)Se 1	/222. LP*(6)Ag 13	2.81	0.89	0.045
195. LP (1)Se 1	/733. BD*(1)Se 1 -Ag 13	2.26	0.81	0.039
197. LP (2)Se 2	/739. BD*(1)Se 4 -Se 10	2.85	0.30	0.027
197. LP (2)Se 2	/744. BD*(1)Se 8 -Se 12	2.85	0.30	0.027
199. LP (2)Se 3	/362. RY*(1)Se 5	1.67	0.75	0.033
199. LP (2)Se 3	/482. RY*(1)Se 9	2.70	0.74	0.042
199. LP (2)Se 3	/732. BD*(1)Se 1 -Se 9	10.31	0.20	0.041
199. LP (2)Se 3	/740. BD*(1)Se 5 -Se 11	6.60	0.24	0.036
201. LP (2)Se 4	/735. BD*(1)Se 2 -Se 10	3.59	0.29	0.029
201. LP (2)Se 4	/741. BD*(1)Se 6 -Se 12	3.49	0.25	0.027
203. LP (2)Se 5	/737. BD*(1)Se 3 -Se 9	2.85	0.30	0.027
203. LP (2)Se 5	/743. BD*(1)Se 7 -Se 11	2.85	0.30	0.027
204. LP (1)Se 6	/222. LP*(6)Ag 13	2.81	0.89	0.045
204. LP (1)Se 6	/742. BD*(1)Se 6 -Ag 13	2.26	0.81	0.039
206. LP (2)Se 7	/732. BD*(1)Se 1 -Se 9	3.49	0.25	0.027
206. LP (2)Se 7	/740. BD*(1)Se 5 -Se 11	3.59	0.29	0.029
208. LP (2)Se 8	/272. RY*(1)Se 2	1.67	0.75	0.033
208. LP (2)Se 8	/572. RY*(1)Se 12	2.70	0.74	0.042
208. LP (2)Se 8	/735. BD*(1)Se 2 -Se 10	6.60	0.24	0.036
208. LP (2)Se 8	/741. BD*(1)Se 6 -Se 12	10.31	0.20	0.041
210. LP (2)Se 9	/731. BD*(1)Se 1 -Se 7	3.49	0.25	0.027
210. LP (2)Se 9	/736. BD*(1)Se 3 -Se 5	3.59	0.29	0.029
212. LP (2)Se 10	/272. RY*(1)Se 2	1.67	0.75	0.033
212. LP (2)Se 10	/332. RY*(1)Se 4	2.70	0.74	0.042
212. LP (2)Se 10	/734. BD*(1)Se 2 -Se 8	6.60	0.24	0.036
212. LP (2)Se 10	/738. BD*(1)Se 4 -Se 6	10.31	0.20	0.041
214. LP (2)Se 11	/362. RY*(1)Se 5	1.67	0.75	0.033
214. LP (2)Se 11	/422. RY*(1)Se 7	2.70	0.74	0.042
214. LP (2)Se 11	/731. BD*(1)Se 1 -Se 7	10.31	0.20	0.041
214. LP (2)Se 11	/736. BD*(1)Se 3 -Se 5	6.60	0.24	0.036
216. LP (2)Se 12	/734. BD*(1)Se 2 -Se 8	3.59	0.29	0.029
216. LP (2)Se 12	/738. BD*(1)Se 4 -Se 6	3.49	0.25	0.027
1. BD (1)Se 1 -Se 7	/232. LP*(9)Ag 14	1.24	0.68	0.026
2. BD (1)Se 1 -Se 9	/232. LP*(9)Ag 14	1.24	0.68	0.026
6. BD (1)Se 3 -Se 5	/229. LP*(6)Ag 14	1.44	0.49	0.025
6. BD (1)Se 3 -Se 5	/230. LP*(7)Ag 14	1.04	0.61	0.023
6. BD (1)Se 3 -Se 5	/232. LP*(9)Ag 14	1.78	0.66	0.031
7. BD (1)Se 3 -Se 9	/229. LP*(6)Ag 14	1.19	0.51	0.024
7. BD (1)Se 3 -Se 9	/231. LP*(8)Ag 14	1.11	0.62	0.024
7. BD (1)Se 3 -Se 9	/232. LP*(9)Ag 14	1.37	0.68	0.027
10. BD (1)Se 5 -Se 11	/229. LP*(6)Ag 14	1.44	0.49	0.025
10. BD (1)Se 5 -Se 11	/230. LP*(7)Ag 14	1.04	0.61	0.023
10. BD (1)Se 5 -Se 11	/232. LP*(9)Ag 14	1.78	0.66	0.031
13. BD (1)Se 7 -Se 11	/229. LP*(6)Ag 14	1.19	0.51	0.024
13. BD (1)Se 7 -Se 11	/231. LP*(8)Ag 14	1.11	0.62	0.024
13. BD (1)Se 7 -Se 11	/232. LP*(9)Ag 14	1.37	0.68	0.027
45. CR (3)Se 3	/232. LP*(9)Ag 14	1.33	10.60	0.106
73. CR (3)Se 5	/229. LP*(6)Ag 14	3.46	10.69	0.185
73. CR (3)Se 5	/230. LP*(7)Ag 14	3.73	10.82	0.181
73. CR (3)Se 5	/232. LP*(9)Ag 14	2.51	10.86	0.148
101. CR (3)Se 7	/229. LP*(6)Ag 14	2.44	10.64	0.155
101. CR (3)Se 7	/231. LP*(8)Ag 14	2.33	10.75	0.142
101. CR (3)Se 7	/232. LP*(9)Ag 14	1.85	10.81	0.127
129. CR (3)Se 9	/229. LP*(6)Ag 14	2.44	10.64	0.155
129. CR (3)Se 9	/231. LP*(8)Ag 14	2.33	10.75	0.142
129. CR (3)Se 9	/232. LP*(9)Ag 14	1.85	10.81	0.127
157. CR (3)Se 11	/232. LP*(9)Ag 14	1.33	10.60	0.106
195. LP (1)Se 1	/232. LP*(9)Ag 14	1.22	0.87	0.029
198. LP (1)Se 3	/229. LP*(6)Ag 14	1.67	0.75	0.034
198. LP (1)Se 3	/232. LP*(9)Ag 14	2.11	0.92	0.039
202. LP (1)Se 5	/229. LP*(6)Ag 14	7.01	0.74	0.069
202. LP (1)Se 5	/230. LP*(7)Ag 14	6.54	0.86	0.067
202. LP (1)Se 5	/232. LP*(9)Ag 14	3.26	0.91	0.049
203. LP (2)Se 5	/229. LP*(6)Ag 14	38.23	0.30	0.098

203.	LP (	2)Se	5		/230.	LP*(	7)Ag	14	7.26	0.42	0.051
203.	LP (	2)Se	5		/232.	LP*(	9)Ag	14	1.52	0.47	0.025
203.	LP (	2)Se	5		/647.	RY*(	3)Ag	14	3.16	2.30	0.080
203.	LP (	2)Se	5		/651.	RY*(	7)Ag	14	1.30	3.33	0.061
203.	LP (	2)Se	5		/653.	RY*(	9)Ag	14	3.90	41.13	0.374
205.	LP (	1)Se	7		/229.	LP*(	6)Ag	14	5.22	0.76	0.060
205.	LP (	1)Se	7		/230.	LP*(	7)Ag	14	1.62	0.88	0.034
205.	LP (	1)Se	7		/231.	LP*(	8)Ag	14	4.21	0.87	0.054
205.	LP (	1)Se	7		/232.	LP*(	9)Ag	14	2.57	0.93	0.044
206.	LP (	2)Se	7		/229.	LP*(	6)Ag	14	22.14	0.29	0.075
206.	LP (	2)Se	7		/230.	LP*(	7)Ag	14	1.40	0.42	0.022
206.	LP (	2)Se	7		/231.	LP*(	8)Ag	14	3.64	0.41	0.035
206.	LP (	2)Se	7		/232.	LP*(	9)Ag	14	1.12	0.47	0.021
206.	LP (	2)Se	7		/647.	RY*(	3)Ag	14	1.33	2.30	0.051
206.	LP (	2)Se	7		/653.	RY*(	9)Ag	14	1.76	41.13	0.249
209.	LP (	1)Se	9		/229.	LP*(	6)Ag	14	5.22	0.76	0.060
209.	LP (	1)Se	9		/230.	LP*(	7)Ag	14	1.62	0.88	0.034
209.	LP (	1)Se	9		/231.	LP*(	8)Ag	14	4.21	0.87	0.054
209.	LP (	1)Se	9		/232.	LP*(	9)Ag	14	2.57	0.93	0.044
210.	LP (	2)Se	9		/229.	LP*(	6)Ag	14	22.14	0.29	0.075
210.	LP (	2)Se	9		/230.	LP*(	7)Ag	14	1.40	0.42	0.022
210.	LP (	2)Se	9		/231.	LP*(	8)Ag	14	3.64	0.41	0.035
210.	LP (	2)Se	9		/232.	LP*(	9)Ag	14	1.12	0.47	0.021
210.	LP (	2)Se	9		/647.	RY*(	3)Ag	14	1.33	2.30	0.051
210.	LP (	2)Se	9		/653.	RY*(	9)Ag	14	1.76	41.13	0.249
213.	LP (	1)Se	11		/229.	LP*(	6)Ag	14	1.67	0.75	0.034
213.	LP (	1)Se	11		/232.	LP*(	9)Ag	14	2.11	0.92	0.039
4.	BD (	1)Se	2	-Se 8	/238.	LP*(	6)Ag	15	1.44	0.49	0.025
4.	BD (	1)Se	2	-Se 8	/239.	LP*(	7)Ag	15	1.04	0.61	0.023
4.	BD (	1)Se	2	-Se 8	/241.	LP*(	9)Ag	15	1.78	0.66	0.031
5.	BD (	1)Se	2	-Se 10	/238.	LP*(	6)Ag	15	1.44	0.49	0.025
5.	BD (	1)Se	2	-Se 10	/239.	LP*(	7)Ag	15	1.04	0.61	0.023
5.	BD (	1)Se	2	-Se 10	/241.	LP*(	9)Ag	15	1.78	0.66	0.031
8.	BD (	1)Se	4	-Se 6	/241.	LP*(	9)Ag	15	1.24	0.68	0.026
9.	BD (	1)Se	4	-Se 10	/238.	LP*(	6)Ag	15	1.19	0.51	0.024
9.	BD (	1)Se	4	-Se 10	/240.	LP*(	8)Ag	15	1.11	0.62	0.024
9.	BD (	1)Se	4	-Se 10	/241.	LP*(	9)Ag	15	1.37	0.68	0.027
11.	BD (	1)Se	6	-Se 12	/241.	LP*(	9)Ag	15	1.24	0.68	0.026
14.	BD (	1)Se	8	-Se 12	/238.	LP*(	6)Ag	15	1.19	0.51	0.024
14.	BD (	1)Se	8	-Se 12	/240.	LP*(	8)Ag	15	1.11	0.62	0.024
14.	BD (	1)Se	8	-Se 12	/241.	LP*(	9)Ag	15	1.37	0.68	0.027
31.	CR (	3)Se	2		/238.	LP*(	6)Ag	15	3.46	10.69	0.185
31.	CR (	3)Se	2		/239.	LP*(	7)Ag	15	3.73	10.82	0.181
31.	CR (	3)Se	2		/241.	LP*(	9)Ag	15	2.51	10.86	0.148
59.	CR (	3)Se	4		/238.	LP*(	6)Ag	15	2.44	10.64	0.155
59.	CR (	3)Se	4		/240.	LP*(	8)Ag	15	2.33	10.75	0.142
59.	CR (	3)Se	4		/241.	LP*(	9)Ag	15	1.85	10.81	0.127
115.	CR (	3)Se	8		/241.	LP*(	9)Ag	15	1.33	10.60	0.106
143.	CR (	3)Se	10		/241.	LP*(	9)Ag	15	1.33	10.60	0.106
171.	CR (	3)Se	12		/238.	LP*(	6)Ag	15	2.44	10.64	0.155
171.	CR (	3)Se	12		/240.	LP*(	8)Ag	15	2.33	10.75	0.142
171.	CR (	3)Se	12		/241.	LP*(	9)Ag	15	1.85	10.81	0.127
196.	LP (	1)Se	2		/238.	LP*(	6)Ag	15	7.01	0.74	0.069
196.	LP (	1)Se	2		/239.	LP*(	7)Ag	15	6.54	0.86	0.067
196.	LP (	1)Se	2		/241.	LP*(	9)Ag	15	3.26	0.91	0.049
197.	LP (	2)Se	2		/238.	LP*(	6)Ag	15	38.23	0.30	0.098
197.	LP (	2)Se	2		/239.	LP*(	7)Ag	15	7.26	0.42	0.051
197.	LP (	2)Se	2		/241.	LP*(	9)Ag	15	1.52	0.47	0.025
197.	LP (	2)Se	2		/690.	RY*(	3)Ag	15	3.16	2.30	0.080
197.	LP (	2)Se	2		/694.	RY*(	7)Ag	15	1.30	3.33	0.061
197.	LP (	2)Se	2		/696.	RY*(	9)Ag	15	3.90	41.13	0.374
200.	LP (	1)Se	4		/238.	LP*(	6)Ag	15	5.22	0.76	0.060
200.	LP (	1)Se	4		/239.	LP*(	7)Ag	15	1.62	0.88	0.034
200.	LP (	1)Se	4		/240.	LP*(	8)Ag	15	4.21	0.87	0.054
200.	LP (	1)Se	4		/241.	LP*(	9)Ag	15	2.57	0.93	0.044
201.	LP (	2)Se	4		/238.	LP*(	6)Ag	15	22.14	0.29	0.075
201.	LP (	2)Se	4		/239.	LP*(	7)Ag	15	1.40	0.42	0.022
201.	LP (	2)Se	4		/240.	LP*(	8)Ag	15	3.64	0.41	0.035
201.	LP (	2)Se	4		/241.	LP*(	9)Ag	15	1.12	0.47	0.021
201.	LP (	2)Se	4		/690.	RY*(	3)Ag	15	1.33	2.30	0.051
201.	LP (	2)Se	4		/696.	RY*(	9)Ag	15	1.76	41.13	0.249
204.	LP (	1)Se	6		/241.	LP*(	9)Ag	15	1.22	0.87	0.029
207.	LP (	1)Se	8		/238.	LP*(	6)Ag	15	1.67	0.75	0.034
207.	LP (	1)Se	8		/241.	LP*(	9)Ag	15	2.11	0.92	0.039
211.	LP (	1)Se	10		/238.	LP*(	6)Ag	15	1.67	0.75	0.034
211.	LP (	1)Se	10		/241.	LP*(	9)Ag	15	2.11	0.92	0.039
215.	LP (	1)Se	12		/238.	LP*(	6)Ag	15	5.22	0.76	0.060
215.	LP (	1)Se	12		/239.	LP*(	7)Ag	15	1.62	0.88	0.034
215.	LP (	1)Se	12		/240.	LP*(	8)Ag	15	4.21	0.87	0.054
215.	LP (	1)Se	12		/241.	LP*(	9)Ag	15	2.57	0.93	0.044
216.	LP (	2)Se	12		/238.	LP*(	6)Ag	15	22.14	0.29	0.075
216.	LP (	2)Se	12		/239.	LP*(	7)Ag	15	1.40	0.42	0.022

216. LP (2)Se	12	/240. LP*(8)Ag	15			3.64	0.41	0.035
216. LP (2)Se	12	/241. LP*(9)Ag	15			1.12	0.47	0.021
216. LP (2)Se	12	/690. RY*(3)Ag	15			1.33	2.30	0.051
216. LP (2)Se	12	/696. RY*(9)Ag	15			1.76	41.13	0.249
229. LP*(6)Ag	14	/370. RY*(9)Se	5			1.52	0.63	0.073
229. LP*(6)Ag	14	/733. BD*(1)Se	1	-Ag	13	1.92	0.11	0.031
229. LP*(6)Ag	14	/232. LP*(9)Ag	14			5.62	0.17	0.073
229. LP*(6)Ag	14	/647. RY*(3)Ag	14			4.87	2.01	0.235
229. LP*(6)Ag	14	/651. RY*(7)Ag	14			3.52	3.03	0.246
229. LP*(6)Ag	14	/652. RY*(8)Ag	14			2.74	2.60	0.201
229. LP*(6)Ag	14	/653. RY*(9)Ag	14			6.60	40.84	1.234
229. LP*(6)Ag	14	/661. RY*(17)Ag	14			1.11	1.09	0.083
229. LP*(6)Ag	14	/677. RY*(33)Ag	14			1.26	1.93	0.118
238. LP*(6)Ag	15	/280. RY*(9)Se	2			1.52	0.63	0.073
238. LP*(6)Ag	15	/742. BD*(1)Se	6	-Ag	13	1.92	0.11	0.031
238. LP*(6)Ag	15	/241. LP*(9)Ag	15			5.62	0.17	0.073
238. LP*(6)Ag	15	/690. RY*(3)Ag	15			4.87	2.01	0.235
238. LP*(6)Ag	15	/694. RY*(7)Ag	15			3.52	3.03	0.246
238. LP*(6)Ag	15	/695. RY*(8)Ag	15			2.74	2.60	0.201
238. LP*(6)Ag	15	/696. RY*(9)Ag	15			6.60	40.84	1.234
238. LP*(6)Ag	15	/704. RY*(17)Ag	15			1.11	1.09	0.083
238. LP*(6)Ag	15	/720. RY*(33)Ag	15			1.26	1.93	0.118

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. Se	0.0000	0.0001	0.0953	0.0017	0.0100	0.0317	0.9302	0.0019	0.9302
2. Se	0.0001	0.0000	0.0000	0.0699	0.0000	0.0100	0.0000	1.0102	0.0000
3. Se	0.0953	0.0000	0.0000	0.0001	1.0102	0.0019	0.0140	0.0001	1.0695
4. Se	0.0017	0.0699	0.0001	0.0000	0.0000	0.9302	0.0005	0.0140	0.0001
5. Se	0.0100	0.0000	1.0102	0.0000	0.0000	0.0001	0.0699	0.0000	0.0699
6. Se	0.0317	0.0100	0.0019	0.9302	0.0001	0.0000	0.0017	0.0953	0.0017
7. Se	0.9302	0.0000	0.0140	0.0005	0.0699	0.0017	0.0000	0.0001	0.0745
8. Se	0.0019	1.0102	0.0001	0.0140	0.0000	0.0953	0.0001	0.0000	0.0001
9. Se	0.9302	0.0000	1.0695	0.0001	0.0699	0.0017	0.0745	0.0001	0.0000
10. Se	0.0019	1.0102	0.0002	1.0695	0.0000	0.0953	0.0001	0.0884	0.0001
11. Se	0.0953	0.0000	0.0884	0.0001	1.0102	0.0019	1.0695	0.0002	0.0140
12. Se	0.0017	0.0699	0.0001	0.0745	0.0000	0.9302	0.0001	1.0695	0.0005
13. Ag	0.3562	0.0012	0.0170	0.0148	0.0012	0.3562	0.0148	0.0170	0.0148
14. Ag	0.0229	0.0001	0.0346	0.0001	0.2387	0.0002	0.1653	0.0000	0.1653
15. Ag	0.0002	0.2387	0.0000	0.1653	0.0001	0.0229	0.0001	0.0346	0.0001

Atom	10	11	12	13	14	15
1. Se	0.0019	0.0953	0.0017	0.3562	0.0229	0.0002
2. Se	1.0102	0.0000	0.0699	0.0012	0.0001	0.2387
3. Se	0.0002	0.0884	0.0001	0.0170	0.0346	0.0000
4. Se	1.0695	0.0001	0.0745	0.0148	0.0001	0.1653
5. Se	0.0000	1.0102	0.0000	0.0012	0.2387	0.0001
6. Se	0.0953	0.0019	0.9302	0.3562	0.0002	0.0229
7. Se	0.0001	1.0695	0.0001	0.0148	0.1653	0.0001
8. Se	0.0884	0.0002	1.0695	0.0170	0.0000	0.0346
9. Se	0.0001	0.0140	0.0005	0.0148	0.1653	0.0001
10. Se	0.0000	0.0001	0.0140	0.0170	0.0000	0.0346
11. Se	0.0001	0.0000	0.0001	0.0170	0.0346	0.0000
12. Se	0.0140	0.0001	0.0000	0.0148	0.0001	0.1653
13. Ag	0.0170	0.0170	0.0148	0.0000	0.0031	0.0031
14. Ag	0.0000	0.0346	0.0001	0.0031	0.0000	0.0000
15. Ag	0.0346	0.0000	0.1653	0.0031	0.0000	0.0000

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
1	se	-0.04368	27.99931	5.98525	0.05911	34.04368
2	se	0.02905	27.99931	5.90451	0.06713	33.97095
3	se	0.18591	27.99931	5.76648	0.04831	33.81409
4	se	0.03567	27.99932	5.90741	0.05760	33.96433
5	se	0.02905	27.99931	5.90451	0.06713	33.97095
6	se	-0.04368	27.99931	5.98525	0.05911	34.04368
7	se	0.03567	27.99932	5.90741	0.05760	33.96433
8	se	0.18591	27.99931	5.76648	0.04831	33.81409
9	se	0.03567	27.99932	5.90741	0.05760	33.96433
10	se	0.18591	27.99931	5.76648	0.04831	33.81409
11	se	0.18591	27.99931	5.76648	0.04831	33.81409
12	se	0.03567	27.99932	5.90741	0.05760	33.96433
13	ag	0.62977	7.99858	10.36047	0.01118	18.37023
14	ag	0.75659	7.99923	10.22338	0.02080	18.24341
15	ag	0.75659	7.99923	10.22338	0.02080	18.24341

```
 * Total *        3.00000   359.98879   101.28233     0.72888   462.00000

For all atoms:
Core                    359.98879(  99.9969% of  360)
Valence                 101.28233(  99.2964% of  102)
Natural Minimal Basis   461.27112(  99.8422% of  462)
Natural Rydberg Basis     0.72888(   0.1578% of  462)

*************************************************************************
*                                                                       *
*              atomic charges with multicenter corrections              *
*                                                                       *
*************************************************************************

                        -------------------------
                           atom   |     charge
                        -------------------------
                            1 se  |    0.1797
                            2 se  |    0.2410
                            3 se  |    0.1597
                            4 se  |    0.1293
                            5 se  |    0.2410
                            6 se  |    0.1797
                            7 se  |    0.1293
                            8 se  |    0.1597
                            9 se  |    0.1293
                           10 se  |    0.1597
                           11 se  |    0.1597
                           12 se  |    0.1293
                           13 ag  |    0.2806
                           14 ag  |    0.3609
                           15 ag  |    0.3609
                        -------------------------
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$Ag_2Se_6^{2+}$ (**B**)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 1.00 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
100. LP (2)Se 1	/132. RY*(4)Se 1	1.19	0.82	0.029
100. LP (2)Se 1	/398. BD*(1)Se 2 -Se 5	3.30	0.34	0.031
100. LP (2)Se 1	/400. BD*(1)Se 4 -Se 6	3.30	0.34	0.031
102. LP (2)Se 2	/189. RY*(1)Se 3	1.66	0.75	0.033
102. LP (2)Se 2	/249. RY*(1)Se 5	2.67	0.75	0.041
102. LP (2)Se 2	/396. BD*(1)Se 1 -Se 5	9.95	0.20	0.040
102. LP (2)Se 2	/399. BD*(1)Se 3 -Se 6	6.63	0.24	0.036
104. LP (2)Se 3	/398. BD*(1)Se 2 -Se 5	3.01	0.29	0.027
104. LP (2)Se 3	/400. BD*(1)Se 4 -Se 6	3.01	0.29	0.027
106. LP (2)Se 4	/279. RY*(1)Se 6	1.01	0.88	0.028
106. LP (2)Se 4	/396. BD*(1)Se 1 -Se 5	3.52	0.25	0.027
106. LP (2)Se 4	/399. BD*(1)Se 3 -Se 6	3.61	0.29	0.029
108. LP (2)Se 5	/159. RY*(1)Se 2	1.01	0.88	0.028
108. LP (2)Se 5	/395. BD*(1)Se 1 -Se 4	3.52	0.25	0.027
108. LP (2)Se 5	/397. BD*(1)Se 2 -Se 3	3.61	0.29	0.029
110. LP (2)Se 6	/189. RY*(1)Se 3	1.66	0.75	0.033
110. LP (2)Se 6	/219. RY*(1)Se 4	2.67	0.75	0.041
110. LP (2)Se 6	/395. BD*(1)Se 1 -Se 4	9.95	0.20	0.040
110. LP (2)Se 6	/397. BD*(1)Se 2 -Se 3	6.62	0.24	0.036
9. CR (3)Se 1	/116. LP*(6)Ag 7	1.27	10.63	0.108
9. CR (3)Se 1	/117. LP*(7)Ag 7	2.02	10.77	0.132
99. LP (1)Se 1	/116. LP*(6)Ag 7	3.53	0.76	0.048
99. LP (1)Se 1	/117. LP*(7)Ag 7	2.69	0.90	0.044
100. LP (2)Se 1	/116. LP*(6)Ag 7	42.01	0.37	0.113
100. LP (2)Se 1	/117. LP*(7)Ag 7	1.30	0.52	0.024
100. LP (2)Se 1	/312. RY*(4)Ag 7	7.03	2.08	0.114
100. LP (2)Se 1	/314. RY*(6)Ag 7	4.82	3.03	0.114
100. LP (2)Se 1	/316. RY*(8)Ag 7	6.83	38.62	0.483
100. LP (2)Se 1	/317. RY*(9)Ag 7	1.90	2.82	0.069
100. LP (2)Se 1	/318. RY*(10)Ag 7	1.64	2.48	0.060
100. LP (2)Se 1	/321. RY*(13)Ag 7	2.28	1.55	0.056
100. LP (2)Se 1	/322. RY*(14)Ag 7	1.33	2.79	0.057
1. BD (1)Se 1 -Se 4	/128. LP*(9)Ag 8	1.17	0.69	0.025
2. BD (1)Se 1 -Se 5	/128. LP*(9)Ag 8	1.17	0.69	0.025
3. BD (1)Se 2 -Se 3	/125. LP*(6)Ag 8	1.46	0.49	0.026

3.	BD (	1)Se	2	-Se	3	/128.	LP*(	9)Ag	8	1.81	0.68	0.031
4.	BD (	1)Se	2	-Se	5	/125.	LP*(	6)Ag	8	1.30	0.51	0.025
4.	BD (	1)Se	2	-Se	5	/127.	LP*(	8)Ag	8	1.15	0.62	0.024
4.	BD (	1)Se	2	-Se	5	/128.	LP*(	9)Ag	8	1.39	0.70	0.028
5.	BD (	1)Se	3	-Se	6	/125.	LP*(	6)Ag	8	1.46	0.49	0.026
5.	BD (	1)Se	3	-Se	6	/128.	LP*(	9)Ag	8	1.81	0.68	0.031
6.	BD (	1)Se	4	-Se	6	/125.	LP*(	6)Ag	8	1.30	0.51	0.025
6.	BD (	1)Se	4	-Se	6	/127.	LP*(	8)Ag	8	1.15	0.62	0.024
6.	BD (	1)Se	4	-Se	6	/128.	LP*(	9)Ag	8	1.39	0.70	0.028
23.	CR (	3)Se	2			/128.	LP*(	9)Ag	8	1.32	10.62	0.106
37.	CR (	3)Se	3			/125.	LP*(	6)Ag	8	3.48	10.69	0.185
37.	CR (	3)Se	3			/126.	LP*(	7)Ag	8	3.58	10.81	0.177
37.	CR (	3)Se	3			/128.	LP*(	9)Ag	8	2.59	10.88	0.150
51.	CR (	3)Se	4			/125.	LP*(	6)Ag	8	2.64	10.64	0.161
51.	CR (	3)Se	4			/127.	LP*(	8)Ag	8	2.44	10.75	0.145
51.	CR (	3)Se	4			/128.	LP*(	9)Ag	8	1.75	10.83	0.123
65.	CR (	3)Se	5			/125.	LP*(	6)Ag	8	2.64	10.64	0.161
65.	CR (	3)Se	5			/127.	LP*(	8)Ag	8	2.44	10.75	0.145
65.	CR (	3)Se	5			/128.	LP*(	9)Ag	8	1.75	10.83	0.123
79.	CR (	3)Se	6			/128.	LP*(	9)Ag	8	1.32	10.62	0.106
99.	LP (	1)Se	1			/125.	LP*(	6)Ag	8	1.21	0.74	0.029
99.	LP (	1)Se	1			/128.	LP*(	9)Ag	8	1.34	0.92	0.031
101.	LP (	1)Se	2			/125.	LP*(	6)Ag	8	1.77	0.75	0.035
101.	LP (	1)Se	2			/128.	LP*(	9)Ag	8	2.13	0.94	0.040
103.	LP (	1)Se	3			/125.	LP*(	6)Ag	8	7.05	0.74	0.069
103.	LP (	1)Se	3			/126.	LP*(	7)Ag	8	6.39	0.86	0.066
103.	LP (	1)Se	3			/128.	LP*(	9)Ag	8	3.48	0.93	0.051
104.	LP (	2)Se	3			/125.	LP*(	6)Ag	8	36.01	0.30	0.095
104.	LP (	2)Se	3			/126.	LP*(	7)Ag	8	6.96	0.41	0.050
104.	LP (	2)Se	3			/128.	LP*(	9)Ag	8	1.65	0.49	0.026
104.	LP (	2)Se	3			/354.	RY*(	3)Ag	8	3.05	2.25	0.077
104.	LP (	2)Se	3			/359.	RY*(	8)Ag	8	3.73	41.74	0.368
105.	LP (	1)Se	4			/125.	LP*(	6)Ag	8	5.65	0.77	0.063
105.	LP (	1)Se	4			/126.	LP*(	7)Ag	8	1.82	0.88	0.036
105.	LP (	1)Se	4			/127.	LP*(	8)Ag	8	4.42	0.87	0.055
105.	LP (	1)Se	4			/128.	LP*(	9)Ag	8	2.47	0.95	0.043
106.	LP (	2)Se	4			/125.	LP*(	6)Ag	8	22.69	0.30	0.076
106.	LP (	2)Se	4			/126.	LP*(	7)Ag	8	1.45	0.41	0.022
106.	LP (	2)Se	4			/127.	LP*(	8)Ag	8	3.71	0.41	0.036
106.	LP (	2)Se	4			/128.	LP*(	9)Ag	8	1.03	0.49	0.021
106.	LP (	2)Se	4			/354.	RY*(	3)Ag	8	1.48	2.25	0.053
106.	LP (	2)Se	4			/359.	RY*(	8)Ag	8	1.88	41.74	0.259
107.	LP (	1)Se	5			/125.	LP*(	6)Ag	8	5.65	0.77	0.063
107.	LP (	1)Se	5			/126.	LP*(	7)Ag	8	1.82	0.88	0.036
107.	LP (	1)Se	5			/127.	LP*(	8)Ag	8	4.42	0.87	0.055
107.	LP (	1)Se	5			/128.	LP*(	9)Ag	8	2.47	0.95	0.043
108.	LP (	2)Se	5			/125.	LP*(	6)Ag	8	22.67	0.30	0.076
108.	LP (	2)Se	5			/126.	LP*(	7)Ag	8	1.44	0.41	0.022
108.	LP (	2)Se	5			/127.	LP*(	8)Ag	8	3.71	0.41	0.036
108.	LP (	2)Se	5			/128.	LP*(	9)Ag	8	1.03	0.49	0.021
108.	LP (	2)Se	5			/354.	RY*(	3)Ag	8	1.48	2.25	0.053
108.	LP (	2)Se	5			/359.	RY*(	8)Ag	8	1.88	41.74	0.259
109.	LP (	1)Se	6			/125.	LP*(	6)Ag	8	1.77	0.75	0.035
109.	LP (	1)Se	6			/128.	LP*(	9)Ag	8	2.13	0.94	0.040
116.	LP*(	6)Ag	7			/132.	RY*(	4)Se	1	2.98	0.45	0.112
116.	LP*(	6)Ag	7			/133.	RY*(	5)Se	1	1.06	0.55	0.074
116.	LP*(	6)Ag	7			/117.	LP*(	7)Ag	7	2.67	0.14	0.059
116.	LP*(	6)Ag	7			/119.	LP*(	9)Ag	7	1.08	0.43	0.067
116.	LP*(	6)Ag	7			/312.	RY*(	4)Ag	7	9.41	1.71	0.391
116.	LP*(	6)Ag	7			/314.	RY*(	6)Ag	7	6.16	2.66	0.394
116.	LP*(	6)Ag	7			/316.	RY*(	8)Ag	7	7.67	38.24	1.670
116.	LP*(	6)Ag	7			/317.	RY*(	9)Ag	7	2.48	2.45	0.240
116.	LP*(	6)Ag	7			/318.	RY*(	10)Ag	7	2.16	2.11	0.208
116.	LP*(	6)Ag	7			/321.	RY*(	13)Ag	7	3.46	1.17	0.196
116.	LP*(	6)Ag	7			/322.	RY*(	14)Ag	7	1.78	2.42	0.202
125.	LP*(	6)Ag	8			/196.	RY*(	8)Se	3	1.39	0.59	0.069
125.	LP*(	6)Ag	8			/116.	LP*(	6)Ag	7	4.54	0.03	0.021
125.	LP*(	6)Ag	8			/128.	LP*(	9)Ag	8	5.65	0.19	0.077
125.	LP*(	6)Ag	8			/354.	RY*(	3)Ag	8	5.22	1.95	0.243
125.	LP*(	6)Ag	8			/355.	RY*(	4)Ag	8	1.30	0.59	0.067
125.	LP*(	6)Ag	8			/359.	RY*(	8)Ag	8	6.70	41.44	1.271
125.	LP*(	6)Ag	8			/368.	RY*(	17)Ag	8	2.99	3.92	0.261

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8
1. Se	0.0000	0.0966	0.0103	0.9316	0.9317	0.0966	0.2996	0.0249
2. Se	0.0966	0.0000	1.0111	0.0140	1.0672	0.0881	0.0194	0.0349
3. Se	0.0103	1.0111	0.0000	0.0704	0.0704	1.0110	0.0017	0.2281
4. Se	0.9316	0.0140	0.0704	0.0000	0.0751	1.0673	0.0135	0.1671
5. Se	0.9317	1.0672	0.0704	0.0751	0.0000	0.0140	0.0135	0.1670

```
   6. Se  0.0966  0.0881  1.0110  1.0673  0.0140  0.0000  0.0194  0.0349
   7. Ag  0.2996  0.0194  0.0017  0.0135  0.0135  0.0194  0.0000  0.0025
   8. Ag  0.0249  0.0349  0.2281  0.1671  0.1670  0.0349  0.0025  0.0000

Summary of Natural Population Analysis:
                                     Natural Population
                 Natural   -----------------------------------
Atom No          Charge        Core        Valence     Rydberg     Total
-------------------------------------------------------------------------
  1  se          -0.07543    27.99936     6.00941     0.06666    34.07543
  2  se           0.18248    27.99930     5.76975     0.04846    33.81752
  3  se           0.02339    27.99931     5.91125     0.06604    33.97661
  4  se           0.04050    27.99932     5.90152     0.05866    33.95950
  5  se           0.04056    27.99932     5.90147     0.05865    33.95944
  6  se           0.18248    27.99930     5.76976     0.04845    33.81752
  7  ag           0.85302     7.99893    10.14128     0.00678    18.14698
  8  ag           0.75300     7.99923    10.22596     0.02181    18.24700
-------------------------------------------------------------------------
 * Total *        2.00000   183.99408    55.63041     0.37551   240.00000

For all atoms:
Core                    183.99408(  99.9968% of  184)
Valence                  55.63041(  99.3400% of   56)
Natural Minimal Basis   239.62449(  99.8435% of  240)
Natural Rydberg Basis     0.37551(   0.1565% of  240)

**********************************************************************
*                                                                    *
*              atomic charges with multicenter corrections           *
*                                                                    *
**********************************************************************

                        -------------------------
                           atom   |     charge
                        -------------------------
                            1 se  |    0.3577
                            2 se  |    0.1626
                            3 se  |    0.2303
                            4 se  |    0.1456
                            5 se  |    0.1455
                            6 se  |    0.1626
                            7 ag  |    0.4420
                            8 ag  |    0.3538
                        -------------------------
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$Ag_2Se_6(SO_2)_2^{2+}$ **(1)**

```
 Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

     Threshold for printing:   1.00 kcal/mol
    (Intermolecular threshold: 0.05 kcal/mol)
                                                                                 E(2)  E(j)-E(i) F(i,j)
        Donor NBO (i)                    Acceptor NBO (j)                      kcal/mol   a.u.    a.u.
 ================================================================================================================

 120. LP (   2)Se   1              /167. RY*(   7)Se   1                        1.02    1.11    0.031
 120. LP (   2)Se   1              /600. BD*(   1)Se   2 -Se   5                2.65    0.31    0.026
 120. LP (   2)Se   1              /602. BD*(   1)Se   4 -Se   6                2.64    0.31    0.026
 122. LP (   2)Se   2              /221. RY*(   1)Se   3                        1.17    0.81    0.029
 122. LP (   2)Se   2              /281. RY*(   1)Se   5                        1.34    0.84    0.031
 122. LP (   2)Se   2              /598. BD*(   1)Se   1 -Se   5                4.33    0.26    0.031
 122. LP (   2)Se   2              /601. BD*(   1)Se   3 -Se   6                4.29    0.26    0.030
 124. LP (   2)Se   3              /227. RY*(   7)Se   3                        1.07    1.12    0.032
 124. LP (   2)Se   3              /600. BD*(   1)Se   2 -Se   5                2.58    0.31    0.026
 124. LP (   2)Se   3              /602. BD*(   1)Se   4 -Se   6                2.59    0.31    0.026
 126. LP (   2)Se   4              /161. RY*(   1)Se   1                        1.16    0.81    0.028
 126. LP (   2)Se   4              /311. RY*(   1)Se   6                        1.36    0.84    0.031
 126. LP (   2)Se   4              /598. BD*(   1)Se   1 -Se   5                4.33    0.26    0.031
 126. LP (   2)Se   4              /601. BD*(   1)Se   3 -Se   6                4.39    0.26    0.031
 128. LP (   2)Se   5              /161. RY*(   1)Se   1                        1.10    0.82    0.028
 128. LP (   2)Se   5              /191. RY*(   1)Se   2                        1.32    0.85    0.031
 128. LP (   2)Se   5              /597. BD*(   1)Se   1 -Se   4                4.09    0.27    0.030
 128. LP (   2)Se   5              /599. BD*(   1)Se   2 -Se   3                4.13    0.27    0.030
 130. LP (   2)Se   6              /221. RY*(   1)Se   3                        1.09    0.82    0.028
 130. LP (   2)Se   6              /251. RY*(   1)Se   4                        1.30    0.85    0.031
 130. LP (   2)Se   6              /597. BD*(   1)Se   1 -Se   4                4.04    0.27    0.030
 130. LP (   2)Se   6              /599. BD*(   1)Se   2 -Se   3                4.02    0.27    0.030
   1. BD (   1)Se   1 -Se   4     /136. LP*(   6)Ag   7                        1.96    0.50    0.030
   1. BD (   1)Se   1 -Se   4     /137. LP*(   7)Ag   7                        2.06    0.65    0.033
   1. BD (   1)Se   1 -Se   4     /138. LP*(   8)Ag   7                        1.65    0.62    0.029
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2. BD (1)Se 1 -Se 5	/136. LP*(6)Ag 7	1.86	0.49	0.029
2. BD (1)Se 1 -Se 5	/137. LP*(7)Ag 7	2.10	0.65	0.034
2. BD (1)Se 1 -Se 5	/138. LP*(8)Ag 7	1.65	0.62	0.029
3. BD (1)Se 2 -Se 3	/136. LP*(6)Ag 7	1.12	0.50	0.023
3. BD (1)Se 2 -Se 3	/137. LP*(7)Ag 7	2.05	0.65	0.033
4. BD (1)Se 2 -Se 5	/136. LP*(6)Ag 7	1.47	0.50	0.026
4. BD (1)Se 2 -Se 5	/137. LP*(7)Ag 7	2.17	0.65	0.034
4. BD (1)Se 2 -Se 5	/139. LP*(9)Ag 7	1.29	0.60	0.025
5. BD (1)Se 3 -Se 6	/136. LP*(6)Ag 7	1.16	0.49	0.023
5. BD (1)Se 3 -Se 6	/137. LP*(7)Ag 7	2.00	0.65	0.033
6. BD (1)Se 4 -Se 6	/136. LP*(6)Ag 7	1.60	0.50	0.027
6. BD (1)Se 4 -Se 6	/137. LP*(7)Ag 7	2.09	0.65	0.034
6. BD (1)Se 4 -Se 6	/139. LP*(9)Ag 7	1.48	0.60	0.027
15. CR (3)Se 1	/136. LP*(6)Ag 7	4.20	10.67	0.204
15. CR (3)Se 1	/137. LP*(7)Ag 7	2.77	10.82	0.158
15. CR (3)Se 1	/138. LP*(8)Ag 7	5.30	10.79	0.216
29. CR (3)Se 2	/136. LP*(6)Ag 7	2.36	10.62	0.152
29. CR (3)Se 2	/137. LP*(7)Ag 7	3.10	10.77	0.167
29. CR (3)Se 2	/139. LP*(9)Ag 7	2.51	10.73	0.148
43. CR (3)Se 3	/137. LP*(7)Ag 7	1.17	10.83	0.103
57. CR (3)Se 4	/137. LP*(7)Ag 7	1.30	10.77	0.108
71. CR (3)Se 5	/137. LP*(7)Ag 7	1.33	10.78	0.109
85. CR (3)Se 6	/136. LP*(6)Ag 7	2.59	10.63	0.160
85. CR (3)Se 6	/137. LP*(7)Ag 7	2.95	10.78	0.163
85. CR (3)Se 6	/139. LP*(9)Ag 7	2.76	10.73	0.155
119. LP (1)Se 1	/136. LP*(6)Ag 7	7.69	0.73	0.072
119. LP (1)Se 1	/137. LP*(7)Ag 7	3.30	0.88	0.049
119. LP (1)Se 1	/138. LP*(8)Ag 7	9.62	0.85	0.081
120. LP (2)Se 1	/136. LP*(6)Ag 7	41.83	0.31	0.105
120. LP (2)Se 1	/137. LP*(7)Ag 7	3.23	0.46	0.035
120. LP (2)Se 1	/138. LP*(8)Ag 7	8.64	0.43	0.056
120. LP (2)Se 1	/345. RY*(5)Ag 7	1.72	2.52	0.062
120. LP (2)Se 1	/350. RY*(10)Ag 7	1.78	3.14	0.070
120. LP (2)Se 1	/351. RY*(11)Ag 7	1.39	3.69	0.067
120. LP (2)Se 1	/352. RY*(12)Ag 7	2.82	4.45	0.105
120. LP (2)Se 1	/353. RY*(13)Ag 7	2.39	5.16	0.104
120. LP (2)Se 1	/357. RY*(17)Ag 7	3.59	34.19	0.327
121. LP (1)Se 2	/136. LP*(6)Ag 7	5.32	0.76	0.061
121. LP (1)Se 2	/137. LP*(7)Ag 7	4.45	0.91	0.058
121. LP (1)Se 2	/138. LP*(8)Ag 7	1.57	0.88	0.033
121. LP (1)Se 2	/139. LP*(9)Ag 7	5.09	0.87	0.059
122. LP (2)Se 2	/136. LP*(6)Ag 7	20.22	0.27	0.068
122. LP (2)Se 2	/137. LP*(7)Ag 7	3.72	0.42	0.036
122. LP (2)Se 2	/138. LP*(8)Ag 7	1.47	0.39	0.022
122. LP (2)Se 2	/139. LP*(9)Ag 7	4.30	0.38	0.037
122. LP (2)Se 2	/353. RY*(13)Ag 7	1.23	5.11	0.074
122. LP (2)Se 2	/357. RY*(17)Ag 7	1.24	34.15	0.191
123. LP (1)Se 3	/137. LP*(7)Ag 7	1.48	0.88	0.033
125. LP (1)Se 4	/136. LP*(6)Ag 7	1.34	0.76	0.030
125. LP (1)Se 4	/137. LP*(7)Ag 7	1.81	0.91	0.037
125. LP (1)Se 4	/139. LP*(9)Ag 7	1.02	0.87	0.027
127. LP (1)Se 5	/136. LP*(6)Ag 7	1.25	0.76	0.029
127. LP (1)Se 5	/137. LP*(7)Ag 7	1.82	0.91	0.037
129. LP (1)Se 6	/136. LP*(6)Ag 7	5.64	0.76	0.062
129. LP (1)Se 6	/137. LP*(7)Ag 7	4.10	0.91	0.055
129. LP (1)Se 6	/138. LP*(8)Ag 7	1.78	0.88	0.035
129. LP (1)Se 6	/139. LP*(9)Ag 7	5.41	0.86	0.061
130. LP (2)Se 6	/136. LP*(6)Ag 7	22.78	0.28	0.073
130. LP (2)Se 6	/137. LP*(7)Ag 7	3.57	0.43	0.035
130. LP (2)Se 6	/138. LP*(8)Ag 7	1.78	0.40	0.024
130. LP (2)Se 6	/139. LP*(9)Ag 7	4.57	0.38	0.038
130. LP (2)Se 6	/353. RY*(13)Ag 7	1.49	5.12	0.081
130. LP (2)Se 6	/357. RY*(17)Ag 7	1.48	34.15	0.209
1. BD (1)Se 1 -Se 4	/145. LP*(6)Ag 8	1.09	0.49	0.022
1. BD (1)Se 1 -Se 4	/146. LP*(7)Ag 8	2.03	0.65	0.033
2. BD (1)Se 1 -Se 5	/145. LP*(6)Ag 8	1.13	0.49	0.023
2. BD (1)Se 1 -Se 5	/146. LP*(7)Ag 8	1.96	0.65	0.032
3. BD (1)Se 2 -Se 3	/145. LP*(6)Ag 8	1.96	0.49	0.030
3. BD (1)Se 2 -Se 3	/146. LP*(7)Ag 8	2.10	0.65	0.034
3. BD (1)Se 2 -Se 3	/147. LP*(8)Ag 8	1.64	0.62	0.029
4. BD (1)Se 2 -Se 5	/145. LP*(6)Ag 8	1.57	0.50	0.027
4. BD (1)Se 2 -Se 5	/146. LP*(7)Ag 8	2.07	0.65	0.033
4. BD (1)Se 2 -Se 5	/148. LP*(9)Ag 8	1.49	0.60	0.027
5. BD (1)Se 3 -Se 6	/145. LP*(6)Ag 8	1.86	0.49	0.029
5. BD (1)Se 3 -Se 6	/146. LP*(7)Ag 8	2.15	0.65	0.034
5. BD (1)Se 3 -Se 6	/147. LP*(8)Ag 8	1.63	0.62	0.028
6. BD (1)Se 4 -Se 6	/145. LP*(6)Ag 8	1.45	0.50	0.026
6. BD (1)Se 4 -Se 6	/146. LP*(7)Ag 8	2.18	0.65	0.034
6. BD (1)Se 4 -Se 6	/148. LP*(9)Ag 8	1.27	0.60	0.025
15. CR (3)Se 1	/146. LP*(7)Ag 8	1.15	10.82	0.102
29. CR (3)Se 2	/146. LP*(7)Ag 8	1.31	10.77	0.108
43. CR (3)Se 3	/145. LP*(6)Ag 8	4.24	10.68	0.205

43.	CR (	3)Se	3		/146.	LP*(	7)Ag	8		2.85	10.83	0.161
43.	CR (	3)Se	3		/147.	LP*(	8)Ag	8		5.31	10.80	0.216
57.	CR (	3)Se	4		/145.	LP*(	6)Ag	8		2.32	10.62	0.151
57.	CR (	3)Se	4		/146.	LP*(	7)Ag	8		3.11	10.77	0.167
57.	CR (	3)Se	4		/148.	LP*(	9)Ag	8		2.44	10.73	0.145
71.	CR (	3)Se	5		/145.	LP*(	6)Ag	8		2.52	10.62	0.157
71.	CR (	3)Se	5		/146.	LP*(	7)Ag	8		2.90	10.78	0.161
71.	CR (	3)Se	5		/148.	LP*(	9)Ag	8		2.77	10.73	0.155
85.	CR (	3)Se	6		/146.	LP*(	7)Ag	8		1.36	10.78	0.111
119.	LP (	1)Se	1		/146.	LP*(	7)Ag	8		1.45	0.88	0.032
121.	LP (	1)Se	2		/145.	LP*(	6)Ag	8		1.33	0.76	0.030
121.	LP (	1)Se	2		/146.	LP*(	7)Ag	8		1.82	0.91	0.037
121.	LP (	1)Se	2		/148.	LP*(	9)Ag	8		1.02	0.87	0.027
123.	LP (	1)Se	3		/145.	LP*(	6)Ag	8		7.72	0.73	0.072
123.	LP (	1)Se	3		/146.	LP*(	7)Ag	8		3.39	0.88	0.050
123.	LP (	1)Se	3		/147.	LP*(	8)Ag	8		9.62	0.85	0.081
124.	LP (	2)Se	3		/145.	LP*(	6)Ag	8		42.65	0.31	0.106
124.	LP (	2)Se	3		/146.	LP*(	7)Ag	8		3.34	0.46	0.036
124.	LP (	2)Se	3		/147.	LP*(	8)Ag	8		8.65	0.44	0.057
124.	LP (	2)Se	3		/388.	RY*(	5)Ag	8		1.74	2.48	0.061
124.	LP (	2)Se	3		/392.	RY*(	9)Ag	8		1.68	2.96	0.066
124.	LP (	2)Se	3		/394.	RY*(	11)Ag	8		1.41	3.71	0.068
124.	LP (	2)Se	3		/395.	RY*(	12)Ag	8		2.89	4.39	0.105
124.	LP (	2)Se	3		/396.	RY*(	13)Ag	8		2.60	5.35	0.110
124.	LP (	2)Se	3		/400.	RY*(	17)Ag	8		3.71	33.99	0.332
125.	LP (	1)Se	4		/145.	LP*(	6)Ag	8		5.26	0.76	0.060
125.	LP (	1)Se	4		/146.	LP*(	7)Ag	8		4.47	0.91	0.058
125.	LP (	1)Se	4		/147.	LP*(	8)Ag	8		1.67	0.88	0.034
125.	LP (	1)Se	4		/148.	LP*(	9)Ag	8		4.95	0.87	0.058
126.	LP (	2)Se	4		/145.	LP*(	6)Ag	8		19.88	0.27	0.068
126.	LP (	2)Se	4		/146.	LP*(	7)Ag	8		3.70	0.42	0.036
126.	LP (	2)Se	4		/147.	LP*(	8)Ag	8		1.54	0.39	0.023
126.	LP (	2)Se	4		/148.	LP*(	9)Ag	8		4.14	0.38	0.036
126.	LP (	2)Se	4		/396.	RY*(	13)Ag	8		1.26	5.30	0.076
126.	LP (	2)Se	4		/400.	RY*(	17)Ag	8		1.21	33.95	0.188
127.	LP (	1)Se	5		/145.	LP*(	6)Ag	8		5.55	0.76	0.062
127.	LP (	1)Se	5		/146.	LP*(	7)Ag	8		4.04	0.91	0.055
127.	LP (	1)Se	5		/147.	LP*(	8)Ag	8		1.74	0.88	0.035
127.	LP (	1)Se	5		/148.	LP*(	9)Ag	8		5.43	0.86	0.061
128.	LP (	2)Se	5		/145.	LP*(	6)Ag	8		22.06	0.27	0.072
128.	LP (	2)Se	5		/146.	LP*(	7)Ag	8		3.47	0.42	0.035
128.	LP (	2)Se	5		/147.	LP*(	8)Ag	8		1.71	0.39	0.024
128.	LP (	2)Se	5		/148.	LP*(	9)Ag	8		4.53	0.38	0.038
128.	LP (	2)Se	5		/396.	RY*(	13)Ag	8		1.44	5.31	0.081
128.	LP (	2)Se	5		/400.	RY*(	17)Ag	8		1.41	33.95	0.203
129.	LP (	1)Se	6		/145.	LP*(	6)Ag	8		1.25	0.76	0.029
129.	LP (	1)Se	6		/146.	LP*(	7)Ag	8		1.86	0.91	0.037
136.	LP*(	6)Ag	7		/165.	RY*(	5)Se	1		1.60	0.60	0.074
136.	LP*(	6)Ag	7		/167.	RY*(	7)Se	1		1.68	0.80	0.088
136.	LP*(	6)Ag	7		/137.	LP*(	7)Ag	7		2.17	0.15	0.037
136.	LP*(	6)Ag	7		/345.	RY*(	5)Ag	7		3.14	2.21	0.199
136.	LP*(	6)Ag	7		/350.	RY*(	10)Ag	7		3.39	2.82	0.233
136.	LP*(	6)Ag	7		/351.	RY*(	11)Ag	7		2.35	3.38	0.212
136.	LP*(	6)Ag	7		/352.	RY*(	12)Ag	7		4.50	4.13	0.325
136.	LP*(	6)Ag	7		/353.	RY*(	13)Ag	7		5.06	4.84	0.374
136.	LP*(	6)Ag	7		/355.	RY*(	15)Ag	7		1.69	2.46	0.154
136.	LP*(	6)Ag	7		/357.	RY*(	17)Ag	7		5.26	33.88	1.007
136.	LP*(	6)Ag	7		/146.	LP*(	7)Ag	8		3.06	0.15	0.044
136.	LP*(	6)Ag	7		/486.	RY*(	1) O	11		1.17	0.96	0.079
145.	LP*(	6)Ag	8		/225.	RY*(	5)Se	3		1.64	0.60	0.075
145.	LP*(	6)Ag	8		/227.	RY*(	7)Se	3		1.73	0.80	0.089
145.	LP*(	6)Ag	8		/137.	LP*(	7)Ag	7		3.02	0.15	0.044
145.	LP*(	6)Ag	8		/146.	LP*(	7)Ag	8		2.13	0.15	0.037
145.	LP*(	6)Ag	8		/388.	RY*(	5)Ag	8		3.07	2.17	0.195
145.	LP*(	6)Ag	8		/392.	RY*(	9)Ag	8		3.12	2.64	0.216
145.	LP*(	6)Ag	8		/394.	RY*(	11)Ag	8		2.35	3.39	0.213
145.	LP*(	6)Ag	8		/395.	RY*(	12)Ag	8		4.39	4.08	0.319
145.	LP*(	6)Ag	8		/396.	RY*(	13)Ag	8		5.24	5.03	0.387
145.	LP*(	6)Ag	8		/398.	RY*(	15)Ag	8		1.30	2.39	0.133
145.	LP*(	6)Ag	8		/400.	RY*(	17)Ag	8		5.27	33.68	1.004
145.	LP*(	6)Ag	8		/403.	RY*(	20)Ag	8		1.08	2.57	0.126
145.	LP*(	6)Ag	8		/512.	RY*(	1) O	12		1.17	0.96	0.079
9.	BD (	1) S	10 - O	11	/137.	LP*(	7)Ag	7		1.96	1.07	0.042
107.	CR (	2) S	10		/137.	LP*(	7)Ag	7		3.66	9.41	0.170
111.	CR (	1) O	11		/137.	LP*(	7)Ag	7		2.19	19.17	0.187
149.	LP (	1) O	9		/137.	LP*(	7)Ag	7		2.15	0.95	0.041
151.	LP (	1) S	10		/137.	LP*(	7)Ag	7		8.27	0.75	0.071
152.	LP (	1) O	11		/136.	LP*(	6)Ag	7		6.53	0.80	0.069
152.	LP (	1) O	11		/137.	LP*(	7)Ag	7		11.88	0.95	0.096
152.	LP (	1) O	11		/138.	LP*(	8)Ag	7		1.91	0.92	0.038
153.	LP (	2) O	11		/136.	LP*(	6)Ag	7		8.57	0.34	0.050
153.	LP (	2) O	11		/137.	LP*(	7)Ag	7		4.38	0.49	0.042

```
  7. BD (   1) O   9 - S  10        /603. BD*(   1) O   9 - S  10          1.65    0.35    0.023
  8. BD (   2) O   9 - S  10        /605. BD*(   1) S  10 - O  11          1.48    1.32    0.041
  9. BD (   1) S  10 - O  11        /604. BD*(   2) O   9 - S  10          1.39    1.34    0.039
105. CR (   1) O   9               /455. RY*(   3) S  10                  1.27   19.92    0.143
105. CR (   1) O   9               /456. RY*(   4) S  10                  1.02   20.63    0.130
110. CR (   5) S  10               /603. BD*(   1) O   9 - S  10          1.29    5.98    0.085
149. LP (   1) O   9               /456. RY*(   4) S  10                  4.30    2.45    0.092
150. LP (   2) O   9               /453. RY*(   1) S  10                 20.83    1.00    0.132
150. LP (   2) O   9               /605. BD*(   1) S  10 - O  11         25.54    0.65    0.117
152. LP (   1) O  11               /455. RY*(   3) S  10                  1.10    1.74    0.039
152. LP (   1) O  11               /457. RY*(   5) S  10                  2.85    2.35    0.074
152. LP (   1) O  11               /604. BD*(   2) O   9 - S  10          2.05    1.21    0.045
153. LP (   2) O  11               /453. RY*(   1) S  10                 10.22    1.05    0.094
153. LP (   2) O  11               /455. RY*(   3) S  10                  3.50    1.28    0.061
153. LP (   2) O  11               /604. BD*(   2) O   9 - S  10         15.89    0.75    0.099
154. LP (   3) O  11               /454. RY*(   2) S  10                 15.12    1.04    0.122
154. LP (   3) O  11               /459. RY*(   7) S  10                  3.54    0.90    0.055
154. LP (   3) O  11               /603. BD*(   1) O   9 - S  10         59.16    0.26    0.113
603. BD*(   1) O   9 - S  10       /440. RY*(  14) O   9                  1.27    1.59    0.103
603. BD*(   1) O   9 - S  10       /454. RY*(   2) S  10                  8.40    0.78    0.171
603. BD*(   1) O   9 - S  10       /459. RY*(   7) S  10                  4.26    0.63    0.119
605. BD*(   1) S  10 - O  11       /453. RY*(   1) S  10                 14.55    0.35    0.208
605. BD*(   1) S  10 - O  11       /455. RY*(   3) S  10                 10.08    0.58    0.252
605. BD*(   1) S  10 - O  11       /489. RY*(   4) O  11                  1.08    1.27    0.138
605. BD*(   1) S  10 - O  11       /604. BD*(   2) O   9 - S  10          7.58    0.04    0.053
 10. BD (   1) O  12 - S  13       /146. LP*(   7)Ag   8                  1.94    1.07    0.042
112. CR (   1) O  12               /146. LP*(   7)Ag   8                  2.17   19.17    0.187
114. CR (   2) S  13               /146. LP*(   7)Ag   8                  3.68    9.41    0.170
155. LP (   1) O  12               /145. LP*(   6)Ag   8                  6.59    0.80    0.069
155. LP (   1) O  12               /146. LP*(   7)Ag   8                 11.75    0.95    0.095
155. LP (   1) O  12               /147. LP*(   8)Ag   8                  1.93    0.92    0.038
156. LP (   2) O  12               /145. LP*(   6)Ag   8                  8.69    0.34    0.050
156. LP (   2) O  12               /146. LP*(   7)Ag   8                  4.36    0.49    0.042
158. LP (   1) S  13               /146. LP*(   7)Ag   8                  8.29    0.75    0.072
159. LP (   1) O  14               /146. LP*(   7)Ag   8                  2.18    0.95    0.041
 10. BD (   1) O  12 - S  13       /608. BD*(   2) S  13 - O  14          1.39    1.34    0.039
 11. BD (   1) S  13 - O  14       /607. BD*(   1) S  13 - O  14          1.65    0.35    0.023
 12. BD (   2) S  13 - O  14       /606. BD*(   1) O  12 - S  13          1.48    1.32    0.041
117. CR (   5) S  13               /607. BD*(   1) S  13 - O  14          1.29    5.98    0.085
118. CR (   1) O  14               /540. RY*(   3) S  13                  1.27   19.92    0.143
118. CR (   1) O  14               /541. RY*(   4) S  13                  1.02   20.63    0.130
155. LP (   1) O  12               /540. RY*(   3) S  13                  1.10    1.74    0.039
155. LP (   1) O  12               /542. RY*(   5) S  13                  2.85    2.35    0.074
155. LP (   1) O  12               /608. BD*(   2) S  13 - O  14          2.05    1.21    0.045
156. LP (   2) O  12               /538. RY*(   1) S  13                 10.22    1.05    0.094
156. LP (   2) O  12               /540. RY*(   3) S  13                  3.49    1.28    0.061
156. LP (   2) O  12               /608. BD*(   2) S  13 - O  14         15.88    0.75    0.099
157. LP (   3) O  12               /539. RY*(   2) S  13                 15.11    1.04    0.122
157. LP (   3) O  12               /544. RY*(   7) S  13                  3.52    0.90    0.055
157. LP (   3) O  12               /607. BD*(   1) S  13 - O  14         59.18    0.26    0.113
159. LP (   1) O  14               /541. RY*(   4) S  13                  4.30    2.45    0.092
160. LP (   2) O  14               /538. RY*(   1) S  13                 20.81    1.00    0.132
160. LP (   2) O  14               /606. BD*(   1) O  12 - S  13          25.52    0.65    0.117
606. BD*(   1) O  12 - S  13       /515. RY*(   4) O  12                  1.07    1.27    0.137
606. BD*(   1) O  12 - S  13       /538. RY*(   1) S  13                 14.52    0.35    0.208
606. BD*(   1) O  12 - S  13       /540. RY*(   3) S  13                 10.07    0.58    0.252
606. BD*(   1) O  12 - S  13       /608. BD*(   2) S  13 - O  14          7.60    0.04    0.053
607. BD*(   1) S  13 - O  14       /539. RY*(   2) S  13                  8.41    0.78    0.171
607. BD*(   1) S  13 - O  14       /544. RY*(   7) S  13                  4.25    0.63    0.119
607. BD*(   1) S  13 - O  14       /584. RY*(  14) O  14                  1.28    1.60    0.103
```

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. Se	0.0000	0.0799	0.0138	0.9972	0.9943	0.0787	0.2310	0.0166	0.0005
2. Se	0.0799	0.0000	0.9964	0.0138	1.0177	0.0852	0.1545	0.0233	0.0003
3. Se	0.0138	0.9964	0.0000	0.0799	0.0788	0.9932	0.0168	0.2340	0.0001
4. Se	0.9972	0.0138	0.0799	0.0000	0.0853	1.0176	0.0233	0.1533	0.0001
5. Se	0.9943	1.0177	0.0788	0.0853	0.0000	0.0138	0.0226	0.1612	0.0001
6. Se	0.0787	0.0852	0.9932	1.0176	0.0138	0.0000	0.1641	0.0226	0.0004
7. Ag	0.2310	0.1545	0.0168	0.0233	0.0226	0.1641	0.0000	0.0166	0.0339
8. Ag	0.0166	0.0233	0.2340	0.1533	0.1612	0.0226	0.0166	0.0000	0.0001
9. O	0.0005	0.0003	0.0001	0.0001	0.0001	0.0004	0.0339	0.0001	0.0000
10. S	0.0009	0.0008	0.0002	0.0003	0.0002	0.0011	0.0634	0.0001	1.6487
11. O	0.0041	0.0020	0.0004	0.0005	0.0005	0.0022	0.1446	0.0003	0.2539
12. O	0.0004	0.0006	0.0043	0.0019	0.0021	0.0005	0.0003	0.1447	0.0000
13. S	0.0002	0.0003	0.0010	0.0008	0.0011	0.0002	0.0001	0.0636	0.0000
14. O	0.0001	0.0001	0.0005	0.0003	0.0004	0.0001	0.0001	0.0341	0.0000

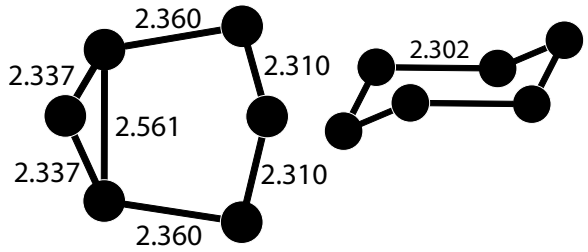
Atom	10	11	12	13	14

```
   1. Se  0.0009  0.0041  0.0004  0.0002  0.0001
   2. Se  0.0008  0.0020  0.0006  0.0003  0.0001
   3. Se  0.0002  0.0004  0.0043  0.0010  0.0005
   4. Se  0.0003  0.0005  0.0019  0.0008  0.0003
   5. Se  0.0002  0.0005  0.0021  0.0011  0.0004
   6. Se  0.0011  0.0022  0.0005  0.0002  0.0001
   7. Ag  0.0634  0.1446  0.0003  0.0001  0.0001
   8. Ag  0.0001  0.0003  0.1447  0.0636  0.0341
   9.  O  1.6487  0.2539  0.0000  0.0000  0.0000
  10.  S  0.0000  1.3557  0.0000  0.0000  0.0000
  11.  O  1.3557  0.0000  0.0000  0.0000  0.0000
  12.  O  0.0000  0.0000  0.0000  1.3560  0.2537
  13.  S  0.0000  0.0000  1.3560  0.0000  1.6478
  14.  O  0.0000  0.0000  0.2537  1.6478  0.0000

Summary of Natural Population Analysis:
                                     Natural Population
                 Natural   ---------------------------------
Atom No          Charge        Core        Valence     Rydberg     Total
           ------------------------------------------------------------
  1  se           0.04647    27.99929     5.89205     0.06220    33.95353
  2  se           0.07719    27.99929     5.86814     0.05538    33.92281
  3  se           0.04549    27.99929     5.89279     0.06243    33.95451
  4  se           0.07776    27.99929     5.86771     0.05524    33.92224
  5  se           0.07137    27.99929     5.87349     0.05585    33.92863
  6  se           0.07041    27.99929     5.87420     0.05610    33.92959
  7  ag           0.74182     7.99900    10.23793     0.02125    18.25818
  8  ag           0.74164     7.99899    10.23822     0.02115    18.25836
  9  o           -0.72742     1.99985     6.68461     0.04295     8.72742
 10  s            1.71003     9.99911     4.09014     0.20071    14.28997
 11  o           -0.91885     1.99985     6.88306     0.03594     8.91885
 12  o           -0.91871     1.99985     6.88291     0.03596     8.91871
 13  s            1.71012     9.99911     4.09011     0.20066    14.28988
 14  o           -0.72732     1.99985     6.68451     0.04296     8.72732
           ------------------------------------------------------------
  * Total *       2.00000   211.99136    91.05987     0.94878   304.00000

For all atoms:
Core                    211.99136(  99.9959% of  212)
Valence                  91.05987(  98.9781% of   92)
Natural Minimal Basis   303.05122(  99.6879% of  304)
Natural Rydberg Basis     0.94878(   0.3121% of  304)

**********************************************************************
*                                                                    *
*              atomic charges with multicenter corrections           *
*                                                                    *
**********************************************************************

                        -------------------------
                           atom   |     charge
                        -------------------------
                            1 se  |    0.2028
                            2 se  |    0.1157
                            3 se  |    0.2061
                            4 se  |    0.1145
                            5 se  |    0.1189
                            6 se  |    0.1210
                            7 ag  |    0.4318
                            8 ag  |    0.4315
                            9 o   |   -0.4364
                           10 s   |    1.1883
                           11 o   |   -0.6236
                           12 o   |   -0.6228
                           13 s   |    1.1882
                           14 o   |   -0.4361
                        -------------------------
```

S4.4 Selenium, Silver and Oxygen distances and angles :Calculated structures on different levels.

	Se6_bp_svp (d3d)	Se6_pbe0_tzvpp (d3d)	Se6_mp2_tzvpp (d3d)	Ag2Se6_1 (BP/SV(P)) A	Ag2Se6_1 (PBE0/TZVPP) A	Ag2Se6_1 ((ri)MP2/tzvpp) A	
Se-Se(Å)	2.381	2.336	2.32	2.408	2.356	2.342	
(in the Se6 ring)							
Se-Se(ave., Å)	2.381	2.336	2.32	2.408	2.356	2.342	
Se-Se-Se(o)	101.74	101.42	100.86				
Se-Se-Se(ave., o)	101.74	101.42	100.86	101.66	101.54	101.14	
Se-Se-Se-Se(ave., o)	75.2	75.71	76.58	75.33	75.52	76.15	
d(Ag1-Se) [Å]				2.933	2.903	2.840	
d(Ag2-Se) [Å]							
d(Ag1-O) [Å]							
	Ag2Se6_2 bp-svp B	Ag2Se6_2 pbe0/tzvpp B	Ag3Se6_2 bp/svp C	Ag3Se6_2 pbe0/tzvpp C	Ag2Se6(SO2)2 pbe0/tzvpp D	Ag2Se6(SO2)2 mp2/tzvpp D	Ag2Se6(SO2)4 pbe0/tzvpp
Se-Se(Å)	2.354 (2x)	2.325 (2x)	2.355 (2x)	2.326 (2x)	2.343 (2x)	2.334 (2x)	2.333 (2x)
(in the Se6 ring)	2.408 (2x)	2.353 (2x)	2.409 (2x)	2.354 (2x)	2.353 (2x)	2.337 (2x)	2.348 (2x)
	2.477 (2x)	2.393 (2x)	2.475 (2x)	2.392 (2x)	2.354 (2x)	2.339 (2x)	2.358 (2x)
Se-Se(ave., Å)	2.413	2.357	2.413	2.357	2.350	2.337	2.347
Se-Se-Se(o)	98.318	99.443 (x2)	97.69	102.91	100.89	100.85	100.56
	100.188	99.617 (x2)	100.41	99.16	100.63	100.82	101.49
	101.202	100.668 (x2)	101.26	100.73	101.79	100.71	100.89
Se-Se-Se(ave., o)	99.90	99.91	99.78	100.93	101.10	100.79	100.98
Se-Se-Se-Se(ave., o)	76.23	76.10	76.04	76.01	76.07	76.67	76.40
d(Ag1-Se) [Å]	2.812	2.756	2.793 (2x)	2.744 (2x)	2.782 (2x)	2.769 (2x)	2.737 (2x)
	2.940 (2x)	2.929 (2x)	2.953 (4x)	2.946 (4x)	3.009 (2x)	2.867 (2x)	3.046 (2x)
					3.045 (2x)	2.918 (2x)	3.295 (2x)
d(Ag2-Se) [Å]	2.568	2.575	2.590 (2x)	2.581			
d(Ag1-O) [Å]					2.258 (2x)	2.224 (2x)	2.358 (2x)
							2.489 (2x)

S4.5 Se_6^{2+} conformers



Se_6^{2+} (boat) Se_6^{2+} (chair)

S5.1 NMR experimental details **1**

Solution NMR ^{19}F-NMR (^{77}Se-NMR) [^{121}Sb-NMR] spectra were obtained using a 10 mm broad-band probe operating at 376.284 (76.391) [95.717] MHz, ^{1}H- and ^{13}C-NMR spectra at 399.947 and 100.578 MHz respectively. ^{19}F-NMR (^{1}H-NMR) spectra were recorded over a shift range of + -240 to +25 ppm (0 to +12 ppm), line-broadening was not applied, typically 32 to 64 transients were accumulated with an acquisition time of 0.60 (3.737) s and a pulse width of 5 (22.3) μs. For each ^{77}Se-NMR sample two spectra were recorded over a shift range of -50 to + 1250 and +1000 to +2100 ppm, line-broadening parameters, used in the exponential multiplication of the free induction decays, were 0 to 40 Hz, further acquisition parameters were as follows: acquisition time, 0.20 s; measuring time in all cases 20 to 60 min or 4000 to 10000 transients. ^{121}Sb-NMR (^{13}C-NMR) spectra were recorded over a shift range of -500 to + 500 ppm (0 to +240 ppm), about 1000 to 3000 (40000 to 60000) transients were acquired for each sample with an acquisition time of 0.20 (1.199) s and a pulse width of 20 (12) μs; line-broadening parameters were 0 to 20 (0) Hz. All NMR-samples were run unlocked, chemical shifts with a positive sign are correlated with shifts to high frequencies (downfield) of the reference compound.

S5.2 Additional Solid State NMR spectra of $(AgI_2)_n$ $nSbF_6$

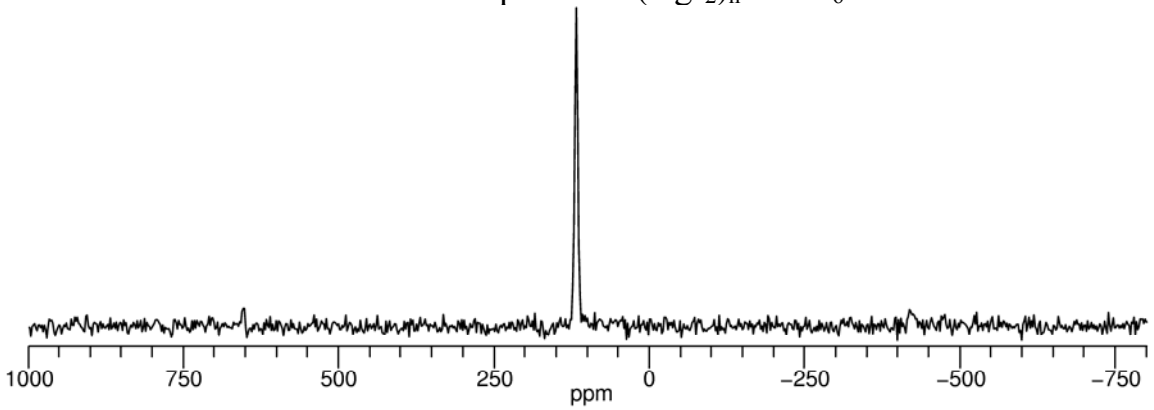


Figure 5.2.1: ^{109}Ag{^{19}F} MAS NMR of $(AgI_2)_n$ $nSbF_6$ obtained with PRESTO-III.

The solid-state ^{19}F NMR spectra are sensitive to the dynamics of SbF_6^- and AsF_6^- anions on the NMR time scale. In liquid-state ^{19}F NMR multiplets caused by J-couplings between ^{19}F and ^{75}As (I = 3/2, 100%), ^{121}Sb (5/2, 57%) or ^{123}Sb (7/2, 43%) are well known.[42] In the solid state NMR, usually only broad lines are observed owing to anisotropic ^{19}F NMR interactions like the magnetic dipole-dipole coupling and the anisotropic chemical shift and the isotropic chemical shift dispersion.[43, 44] The well resolved multiplets in Figure 18 give evidence of fast rotational motion, fast enough too cancel out homonuclear dipolar interactions between ^{19}F nuclei. This is evident by comparing experimental spectra with simulated spectra (not shown) taking into account all direct dipolar interactions within a XF_6 (X = As, Sb) octahedron. We conclude that the rotational motion of XF_6 anions is thermally activated for all samples investigated in this study. Isotropic chemical shift values agree well with those reported in liquid-state NMR. Note that fast and free rotational motion implies that only a single ^{19}F resonance per octahedron is expected. Clearly the two quartets in the ^{19}F NMR spectrum of $AgAsF_6$ give evidence of two crystallographically inequivalent AsF_6 units, which does not agree with the reported description.[45]

Similar observations were made for the solid state ^{19}F-environments in the related salts $Ag(C_2H_4)_3^+[A]^-$ $Ag(P_4S_3)_3^+[A]^-$ with only one sharp ^{19}F MAS-NMR resonance for each anion due to dynamics.[46, 47] Temperature dependent NMR combined with single-crystal X-ray diffraction should be able to lift this contradiction but go beyond the scope of this contribution.

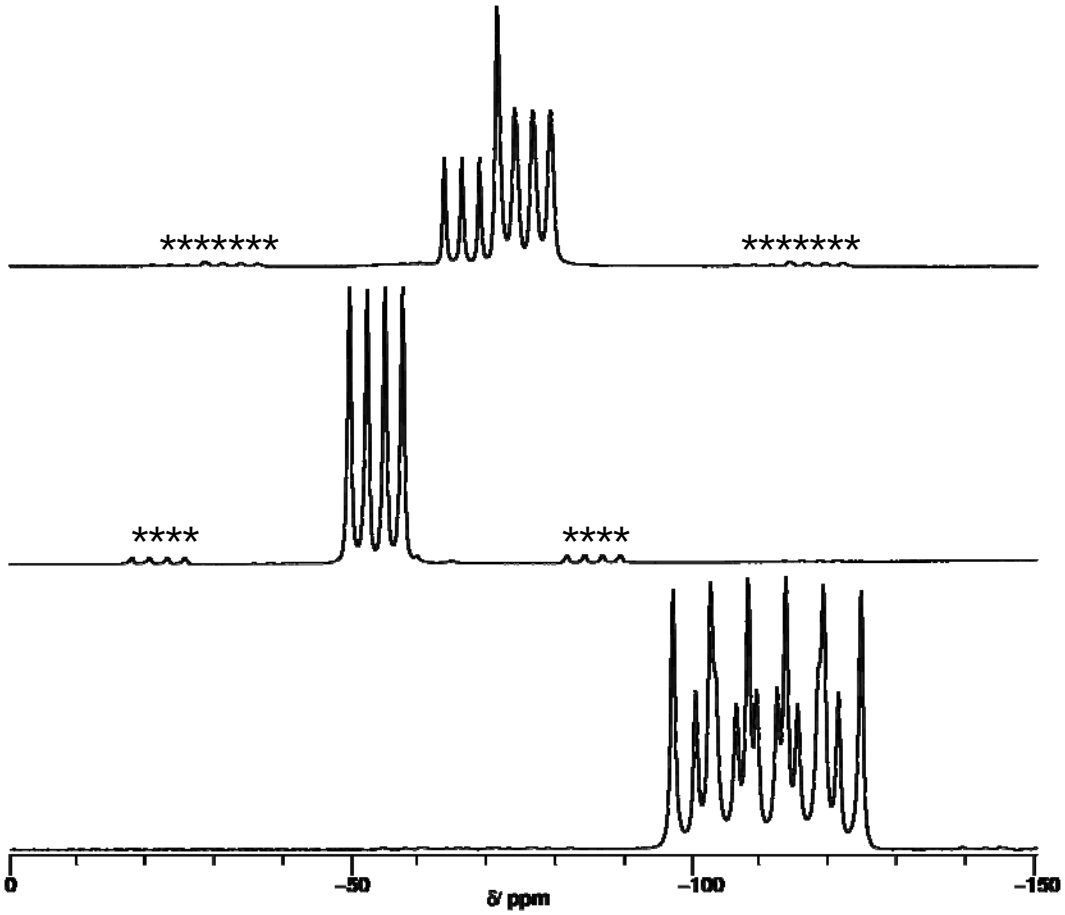


Figure 5.2.2: ^{19}F MAS NMR spectra of $(AgI_2)_n \cdot nSbF_6$ (bottom), $(AgI_2)_n \cdot nAsF_6$ (middle) and $AgAsF_6$ (top) at 16, 12 and 16 kHz rotor spinning frequency, respectively; peaks marked by asterisks are rotational sidebands.

S6 Syntheses of $Ag[Sb(OTeF_5)_6]$

a) With CH_2Cl_2 solvent $Ag[Sb(OTeF_5)_6]$ was initially synthesized according to the literature procedure. However, due to the extreme sensitivity of this compound, the glass vessels were flame dried with SF_4 for at least one hour and flame dry the vessels after the SF_4 treatment. Freshly prepared $AgOTeF_5$ (13.14 g, 37.94 mmol) was weighed into a two bulb-frit plate vessel and exposed over night to a dynamic vacuum to remove all traces of CH_2Cl_2. A stock solution of $SbCl_5$ in F-114 (5.57 ml, 1.326 M, 7.39 mmol) was transferred By a direct connection into the second bulb and approximately 10 ml of F-114 added. This F-114-$SbCl_5$ solution was then poured onto the solid $AgOTeF_5$ A reaction immediately started with warming to about 40^{o}C with a change in the appearance of the precipitate. About 10 ml of

CH_2Cl_2 were added after stirring the suspension over night and a brownish clear solution was given on filtration. The insoluble material was washed six times when all volatiles were removed in vacuo and the remaining solid beige residue was exposed to a dynamic vacuum overnight. The flask was cut open and the soluble material grounded for 5 minutes and transferred into a one bulb vessel (10.60 g vs. 10.50 g expected) and exposed to a dynamic vacuum for 96 hours, during which there was a weight loss of 0.638 g. A NMR-sample of this previously all soluble material (0.30 g) was prepared in SO_2 (approx. 4 g) and revealed the presence of some insoluble beige material. The solution ^{19}F-NMR spectrum showed only lines attributable to the $Sb(OTeF_5)_6^-$ anion, however, in the 1H-NMR spectrum one line at ^{1}H = 5.12 ppm was observed (= CH_2Cl_2). An IR-spectrum of this material did not show the presence of CH_2Cl_2. The solid material (9.299 g) was then exposed for another 130 hours to a dynamic vacuum during which a constant weight loss of 4.6 mg/hour was observed. The grease of the trap of the vacuum line turned black during this time suggesting the evolution of a reactive volatile species. The remaining 8.701 g of beige solid were dissolved in 12.46 g of SO_2 and filtered into a second bulb leaving 0.694 g of a solid, insoluble beige residue. This insoluble material did not dissolve in CH_2Cl_2 with ultrasonic enhancement (NMR) and its FT-Raman spectrum showed the presence of small amounts of $SbCl_6^-$ {possibly from $SbCl_5$ + AgCl → $Ag[SbCl_6]$, RA(cm^{-1}): 330(υ1, 100), 281(υ2, 22), 196(υ5, 31) cm-1(int%) assignments from[33] and a teflate containing substance{ possibly Ag[(O)Sb(OTeF5)4], RA(cm^{-1}): 716(18), 703(16), 666(100), 448(10), 411(5), 395(88), 308(11), 241(14), 164(21), 142(26), 122(19), 105(sh) cm-1(int%)}. A MS only showed fragments attributable to $SbCl_5$(from $Ag[SbCl_6]$). The soluble material was exposed 6 hours to a dynamic vacuum until a (small) constant weight-loss was achieved. The nature of this soluble material was monitored by ^{19}F-and ^{121}Sb-NMR spectroscopy (SO_2 solution) showing the exclusive presence of lines attributable to the $Sb(OTeF_5)_6^-$ anion [δ^{19}F = -40.6 ppm, $^1J(^{19}F,^{125}Te)$ =3563 Hz; δ ^{121}Sb = -12.6 ppm; $^2J(^{121}Sb,^{125}Te)$ = 763 Hz], however in the ^{1}H - NMR still one line attributable to CH_2Cl_2 was observed at δ ^{1}H = 5.12 ppm.

b) With SO_2 solvent A stock solution of $SbCl_5$ in F-114 (5.75 ml, 1.326 M, 7.62 mmol) was transferred by a direct connection into one bulb of a two bulb frit plate vessel and additional 42.61 g F-114 were condensed onto it. This solution was poured onto the solid $AgOTeF_5$ (13.56 g, 39.15 mmol) in a second bulb and vigorously shaken for about 15 min after which the solution was left stirring over night. Addition of 6.76 g of SO_2 led to a slimy, paint like mixture. Filtration resulted in two separate liquid phases: a brownish SO_2 and colourless F-114 phase. The insolubles were extracted 6 times after which all solubles had been transferred into the second bulb. All volatiles were removed in vacuo and the resulting solid was exposed for 24 hours to a dynamic vacuum after which 0.78 g of a volatile material was lost (compared to the initial weight). 5.83 g SO_2 were condensed onto the solubles and filtered into a separate bulb (15.55 g solution transferred) leaving 5.70 g of a insoluble material [calc. AgCl: 4.64 g) and extracting 9.72 g soluble material ($Ag[Sb(OTeF_5)_6]$, yield: 90 %). An ^{19}F-NMR

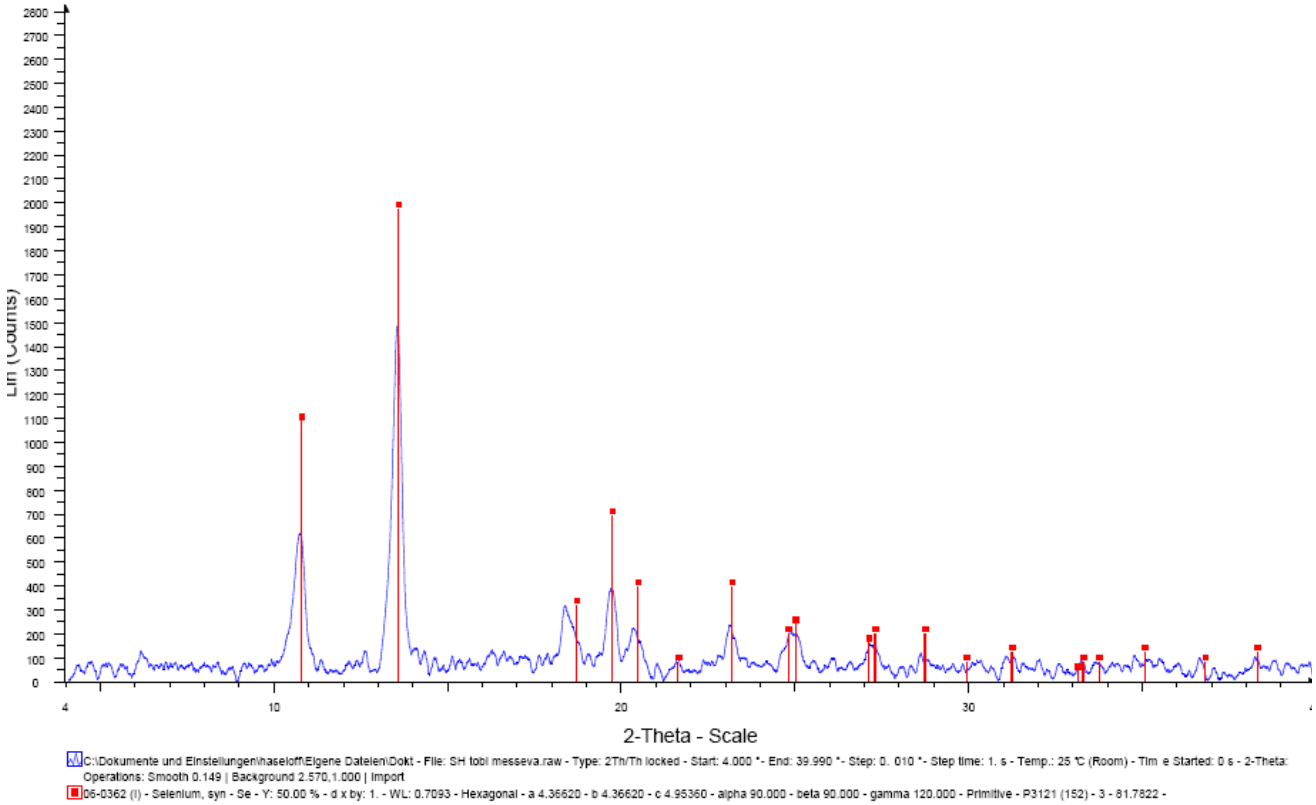
spectrum of the soluble material in SO_2 / SO_2ClF mixture (4 g, 1:3 by weights) confirms the exclusive presence of lines attributable to the $Sb(OTeF_5)_6^-$ anion but the ^1H - NMR spectrum still showed the presence of one line at $\delta\ ^1H = 4.66$ ppm.

S7 Attempted syntheses of $[Se_x][Sb(OTeF_5)_6]$(x = 6, 8)

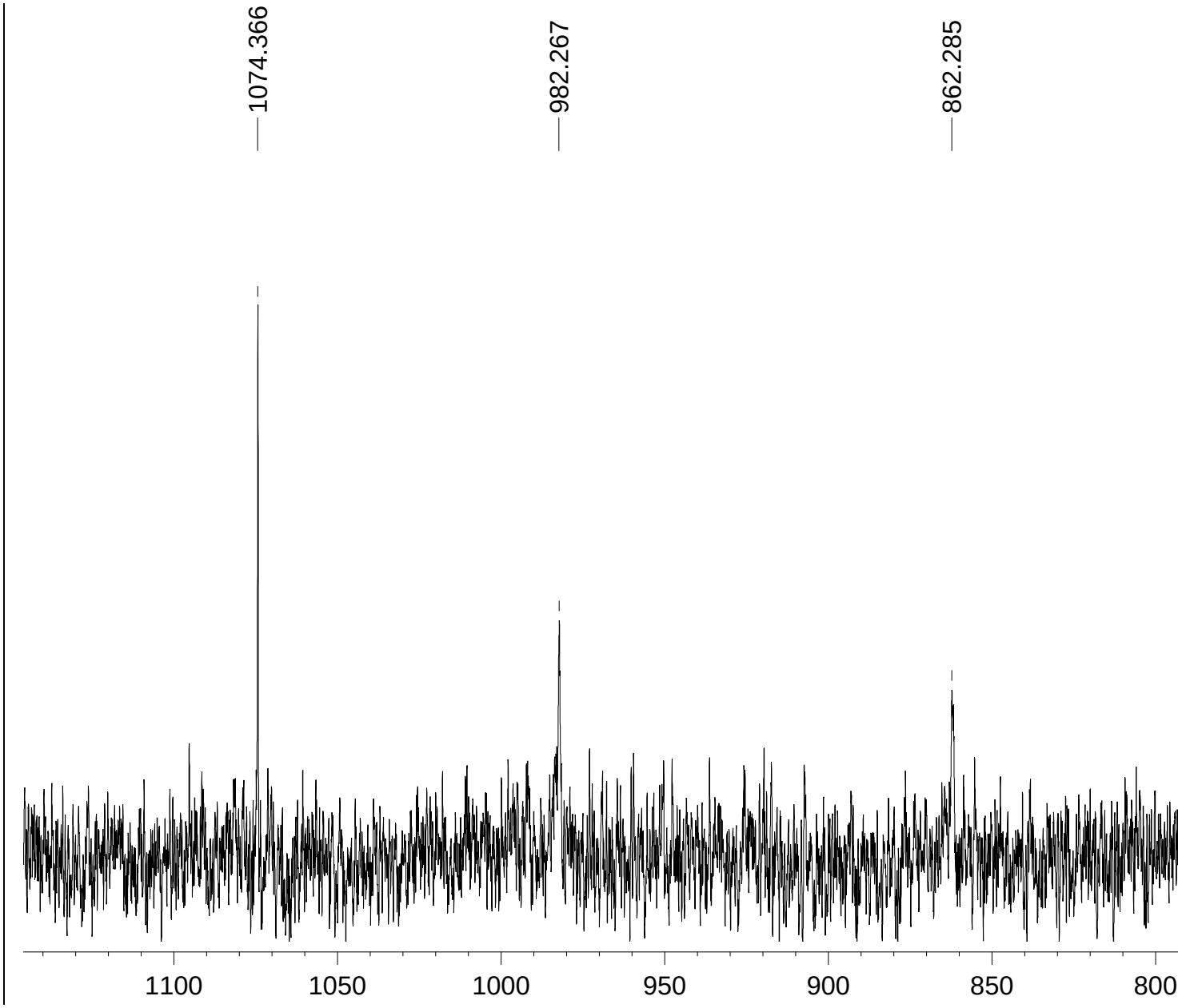
Grey selenium (99.0 %, 0.131 g, 1.653 mmol) and 0.961 g $Ag[Sb(OTeF_5)_6]$ (0.579 mmol) were weighed into a 10 mm (o.d.) thick walled NMR tube, 4 g of SO_2 (5.5 cm height) was added and sonicated one hour at ambient temperature giving a greenish yellowish solution. NMR spectra at 0 ^oC, -30 and -70 ^oC showed two resonances at $\delta\ ^{77}Se$ = 1100±7 and 766±5 ppm [Se_{10}^{2+}] as well as those attributable to the Se_8^{2+} dication in about 10% of the total intensity (only at -70 ^oC, $\delta\ ^{77}Se$ = 1058, 1077, 1205, 1533, 1978 ppm). A preparation using an excess of Se [0.190 g Se (2.409 mmol) and 0.525 g $Ag[Sb(OTeF_5)_6]$ (0.316 mmol) in approx. 4 g of SO_2] gave a similar product (^{77}Se-NMR) and unreacted selenium. In another preparation, a stock solution of $Ag[Sb(OTeF_5)_6]$ in SO_2 (1.6 ml, 0.395 M, 0.632 mmol) was poured onto grey selenium (0.174 g, 2.204 mmol) in a 10 mm NMR tube through a suitable adapter.[A graded cylinder fitted with a J. Young valve and a direct connection (7 mm diameter) suitable to attach a 10 mm NMR tube. The connection includes a Rotoflo valve with a ¼" which is used to flame dry the evacuated direct connection prior to use. To ensure complete transfer of the stock solution, small amounts of the solvent were condensed three times into the cylinder and poured back to the reaction vessel.] About 3-4 g of SO_2 were added to reach the optimum height for NMR measurements (5.5 cm). This mixture was exposed to ultrasonic for one hour at ambient temperature giving a clear, intensely yellow-orange solution over a small amount of black precipitate. NMR spectra at -30 ^oC showed the presence of similar resonances at $\delta\ ^{77}Se$ = 774 and 1071 ppm (as well as unassigned lines at $\delta\ ^{77}Se$ = 879 and 994 ppm). The yellow solution was decanted into a two bulb vessel fitted by a J. Young NMR valve by the direct connection of the NMR-tube and the vessel. 0.061 g of a blackish material [99% Se, FT-Raman] remained in the tube (together with a little yellow solid on the glass walls). Yellow-orange crystals were obtained from the yellow orange SO_2 solution by the application of a temperature gradient (ΔT = 10 - 20 ^oC) at an outside temperature of 5 ^oC.[One bulb of the vessel was placed in a small Dewar vessel which was filled by about 20% with liquid N_2 so that the bottom of the bulb and the surface of the liquid N_2 were separated by approximately 3 to 4 cm.] On removal of the dewar, the block like crystals dissolved very readily, presumably in small amounts of SO_2. Therefore all volatiles were removed in vacuo (1.5 h), while the crystals were cooled to ca. -20 to -30 ^oC, giving 1.19 g {0.361 mmol, 96 % based on $Ag[Sb(OTeF_5)_6]$} crystalline material (slightly sticky). 0.5004 g (0.1296 mmol) of the yellow material were loaded in a 10 mm (o.d.) NMR tube and 3.9761 g of SO_2 condensed onto the sample giving a yellow solution. 0.5218 g (12.7104 mmol) of CH_3CN were then condensed onto the frozen (77 K) solution. Upon warming a red precipitate over a

clear, colourless solution was immediately formed. The acetonitrile methyl groups show only one signal in the proton NMR spectrum (r.t. and -70 ^{o}C). The red material darkened considerably over several weeks and was separated from the clear solution by filtration into a specially designed apparatus. After carefully washing the insoluble material about six times with SO_2, all volatiles were removed in vacuo and the solid material was shown to be elemental selenium (FT-Raman).

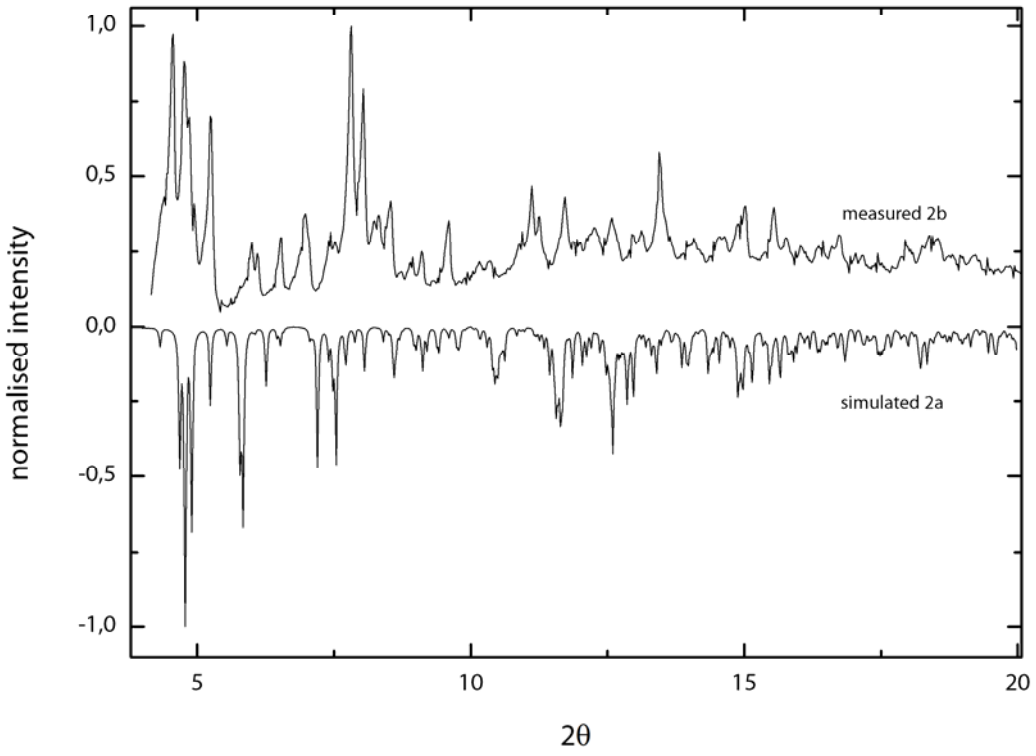
S8 Powder Spectra of the greyish remains in the synthesis of **2** which are confirmed to be grey selenium.



S9 ^{77}Se-spectra of **2** after 27000 scans (5s delay, 0.85s acquisition time) in SO_2 solution in J. Young 5 mm NMR tube.



S10 Power XRD r.t. (Cu).



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15. Some residual electron density can be found close to the Se_6-ring (density max 2.261/ min. -1.355). It is possible to refine an alternative Se8-complex with a occupation of less than 5% in the cation, but there are invariancies in the angles and distances compared to Se_8 (see supplemental). The influence on the all overall quality of the refinement is small e.g. (R1 = 0.1038, wR2 = 0.2654), but more NPDs occur in the anion, leading to an inacceptable data /parameter ratio. Therefore we decided to omit this Se_8-fragment in the final refinement.
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