

The Crystal Structures and Raman Spectra of $2S_8 \cdot SnI_4$ and $2S_n \cdot Se_{8-n} \cdot SnI_4$

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The crystal structures of $2S_8 \cdot SnI_4$ and $2S_n \cdot Se_{8-n} \cdot SnI_4$ were determined from three-dimensional X-ray diffraction data. $2S_8 \cdot SnI_4$ crystallizes in the orthorhombic space group $Fdd2$ with the cell parameters $a=20.885(6)$, $b=21.805(5)$, and $c=11.398(3)$ Å, $Z=8$. $2S_n \cdot Se_{8-n} \cdot SnI_4$ is triclinic with the space group $P1$ and has the cell parameters $a=11.413(6)$, $b=16.137(14)$, $c=8.098(6)$ Å, $\alpha=92.34(7)$, $\beta=110.47(5)$, and $\gamma=68.90(5)^\circ$, $Z=2$. The structures were refined to final R -values of 0.075 and 0.084, respectively. In $2S_8 \cdot SnI_4$ every SnI_4 unit is surrounded by twelve S_8 molecules and conversely every S_8 ring is surrounded by six SnI_4 molecules. In $2S_n \cdot Se_{8-n} \cdot SnI_4$ every tin tetraiodide tetrahedron is surrounded by ten eight-membered rings. Of the two crystallographically independent $S_n \cdot Se_{8-n}$ molecules one is surrounded by six SnI_4 units and the other by four. The closest packing of the sulfur or sulfur–selenium molecules is comparable to that in sulfur allotropes. The Raman spectrum of the sulfur–selenium adduct shows that the compound cannot be stoichiometrically pure $2S_7 \cdot Se \cdot SnI_4$ as reported in the literature since the presence of selenium–selenium bonds is indicated by the spectrum. It is inferred that the adduct consists of different $S_n \cdot Se_{8-n}$ molecules in varying concentrations as is the case in the sulfur–selenium crystals produced by the recrystallization of quenched molten mixtures of the elements.

Binary sulfur–selenium compounds form a very complex system in the solid state. X-Ray investigations^{1–5} have revealed that while the structures consist of eight- and twelve-membered ring molecules the occupation of all atomic sites is statistical owing to the formation of mixed crystals of different $S_n \cdot Se_{8-n}$ or $S_n \cdot Se_{12-n}$ molecules. Recent

Raman spectroscopic investigation of the eight-membered species⁶ suggested that these crystals consist of molecules with adjacent selenium atoms. By comparing the wave numbers calculated for thirteen different $S_n \cdot Se_{8-n}$ molecules to the Raman spectra of four phases obtained by recrystallizing the quenched molten mixtures of sulfur and selenium in varying molar ratios the presence of selenium–selenium bonds in the molecules was confirmed.⁷ These calculations also revealed that structural units of the type S–Se–S are not abundant in the $S_n \cdot Se_{8-n}$ phases in question.

On the other hand, elemental sulfur is known to form adducts with molecular iodides and a weak charge transfer bond is created between the sulfur and the iodine atom. The best characterized adducts are $CHI_3 \cdot 3S_8$ ⁸ and $SbI_3 \cdot 3S_8$.⁹ Hawes^{10,11} has made preliminary X-ray studies of $2S_8 \cdot SnI_4$ and $2S_7 \cdot Se \cdot SnI_4$. The present work was undertaken to obtain structural information about these adducts as a part of a systematic investigation on the structures and composition of sulfur–selenium phases.

EXPERIMENTAL

$2S_8 \cdot SnI_4$ was obtained by dissolving sulfur and tin tetraiodide in the molar ratio of 2:1 in toluene at room temperature and crystallizing the product at $-20^\circ C$. The orange needles formed had a melting point of $101^\circ C$ which is identical to that reported by Hawes.¹⁰ The sulfur–selenium adduct was prepared by melting sulfur and selenium in a molar ratio 6:2. After quenching, the mixture was extracted in boiling toluene and SnI_4 was added to the extract. By cooling to $-20^\circ C$ two kinds of crystals appeared: orange needles of

S_nSe_{8-n} molecules and a few red plate-like crystals of the adduct which had the melting point of 96–98 °C (Hawes: 98 °C¹¹).

The Raman spectra of the adducts and SnI_4 were recorded with a Varian Cary 82 spectrometer equipped with a triple monochromator and a krypton laser (647.1 nm). All spectra were measured at about –120 °C in order to avoid the decomposition of the samples in the laser beam and to obtain better resolution in the spectra.

An automatic Syntex $P2_1$ four-circle diffractometer with graphite monochromatized $MoK\alpha$ radiation was utilized in the determination of the unit cell parameters and in the collection of the intensity data. The unit cell parameters were calculated from the diffractometer measurements of setting angles for 25 ($2S_8SnI_4$) and 15 ($2S_nSe_{8-n}SnI_4$) reflections in the 2θ range of 3–22°, and the data were refined by a least-squares method. The crystal data for both adducts are presented in Table 1. The intensity data were collected with ω -scan technique in the interval $5^\circ < 2\theta < 60^\circ$ by using a variable scan speed from 1 to 30°/min. Of the 2573 ($2S_8SnI_4$) and 5121 ($2S_nSe_{8-n}SnI_4$) independent reflections there were 1637 and 3115 reflections, respectively, which satisfied the criterion $I \geq 2\sigma(I)$. Empirical absorption corrections were made from ψ -scan data after which Lorentz and polarization corrections were applied to both sets of data.

The structures were solved by direct methods using the program MULTAN 78.¹² The positions of I and Sn were determined from 142 E -values (>1.726) and 184 E -values (>2.094) for $2S_8SnI_4$ and $2S_nSe_{8-n}SnI_4$, respectively. These positions were refined using the XRAY 76¹³ program package. The subsequent difference Fourier maps provided the positions of all remaining atoms in both cases. The scattering factors were those of Cromer and Mann¹⁴ for neutral atoms. After five cycles of refinement with isotropic temperature factors the R -values were 0.101 ($2S_8SnI_4$) and 0.144 ($2S_nSe_{8-n}SnI_4$). Further five cycles with anisotropic temperature factors and with allowance for disorder in the case of the sulfur–selenium adduct with the technique reported earlier⁴ led to the final R -values of 0.075 ($2S_8SnI_4$) and 0.084 ($2S_nSe_{8-n}SnI_4$). All calculations were carried out with a UNIVAC 1108 computer. Listings of observed and calculated structure factors are available from the authors upon request.

RESULTS AND DISCUSSION

The unit cell parameters and the space group of $2S_8SnI_4$ (see Table 1) agree closely with those

Table 1. Crystal data for $2S_8SnI_4$ and $2S_nSe_{8-n}SnI_4$.

	$2S_8SnI_4$	$2S_nSe_{8-n}SnI_4$
a (Å)	20.885(6)	11.413(6)
b (Å)	21.805(5)	16.137(14)
c (Å)	11.398(3)	8.098(6)
α (°)	90.0	92.34(7)
β (°)	90.0	110.47(5)
γ (°)	90.0	68.90(5)
V (Å ³)	5190.6	1297.4
Space group	$Fdd2$	$P\bar{1}$
Z	8	2
D_x (g cm ⁻³)	2.916	
$\mu_{MoK\alpha}$ (cm ⁻¹)	69.31	

reported by Hawes.¹⁰ In the case of the sulfur–selenium adduct this is not so straightforward. While it was possible to index the reflections with the parameters $a = 20.311(10)$, $b = 22.363(11)$, $c = 11.424(3)$ Å, $\alpha = 90.37(3)$, $\beta = 89.73(3)$, and $\gamma = 89.70(4)^\circ$ which agree roughly with the orthorhombic lattice parameters given by Hawes,¹¹ no axial symmetry was observed and the unit cell was found to reduce to the triclinic one with the space group $P\bar{1}$ and the parameters presented in Table 1.

The positional and thermal parameters of the atoms are presented in Table 2, bond lengths and angles in Table 3, iodine–sulfur distances in Table 4, and short intermolecular distances in Table 5.

In both compounds SnI_4 forms a fairly regular tetrahedron with average bond lengths and angles of 2.663 Å, 109.5° and 2.669, 109.5° for the sulfur and sulfur–selenium adduct, respectively. The bond length in pure SnI_4 has been reported as 2.69(2) Å assuming the molecule to be a regular tetrahedron.¹⁵ The average SS bond length in $2S_8SnI_4$ is 2.05 Å and the average bond angle 107°. These values are quite normal for S_8 .^{16–18} The average bond length and angle in the ring molecules of the sulfur–selenium adduct are 2.07 Å and 108°, respectively.

The existence of charge-transfer bonds in $CHI_3 \cdot 3S_8$ ⁸ and $SbI_3 \cdot 3S_8$ ⁹ was deduced from the observation of a nearly linear $X-I \cdots S(X=C \text{ or } Sb)$ arrangement with $I-S$ distances of 3.50 and 3.60 Å for the iodoform and antimony tri-iodide adducts, respectively. In neither of the two adducts of tin tetraiodide can a similar charge-transfer bond be found. In both compounds the iodine atoms have close contacts to several atoms of the eight-

Table 2. Atomic coordinates and anisotropic temperature coefficients with their estimated standard deviations. The temperature coefficients are of the form $\exp(-2\pi^2(h^2a^{*2}U_{11} + \dots + 2klb^*c^*U_{23}))$ and have been multiplied by 10^3 .

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A. $2S_8 \cdot SnI_4$									
Sn1	.5	.5	.0	43(6)	33(5)	26(4)	1(6)	0	0
I1	.3942(4)	.4986(5)	.1299(9)	45(4)	59(5)	36(4)	2(5)	7(4)	2(5)
I2	.4964(5)	.6004(4)	-.1332(9)	67(5)	40(4)	38(4)	-0(5)	-0(6)	9(4)
S1	.245(2)	.659(2)	.113(4)	83(28)	48(19)	42(18)	-6(21)	12(25)	0(19)
S2	.266(2)	.608(2)	.262(4)	65(27)	70(26)	33(17)	-8(21)	-1(18)	-7(19)
S3	.179(2)	.580(2)	.329(4)	62(25)	64(25)	36(18)	-21(21)	15(18)	-15(18)
S4	.165(3)	.493(2)	.276(4)	103(37)	48(23)	36(18)	-9(25)	-4(23)	9(18)
S5	.103(2)	.495(2)	.133(4)	68(23)	66(24)	39(17)	-19(23)	-1(21)	-5(23)
S6	.159(2)	.487(2)	-.015(4)	88(31)	36(19)	39(19)	-12(19)	2(21)	-6(15)
S7	.172(2)	.573(2)	-.081(4)	61(24)	63(25)	40(19)	-23(21)	-13(18)	13(18)
S8	.261(2)	.602(2)	-.028(3)	51(23)	73(27)	32(16)	-10(20)	4(16)	1(18)
B. $2S_n Se_{8-n} \cdot SnI_4$									
Sn1	.3511(4)	.2610(2)	.4364(5)	41(2)	45(2)	36(2)	-22(2)	17(1)	-7(1)
I1	.3774(4)	.3539(3)	.1976(5)	57(2)	60(2)	50(2)	-27(2)	25(2)	4(2)
I2	.5909(4)	.1551(3)	.6657(5)	47(2)	58(2)	49(2)	-20(2)	11(2)	-1(2)
I3	.2255(4)	.1545(3)	.2648(5)	60(2)	58(2)	47(2)	-38(2)	15(2)	-12(2)
I4	.2163(4)	.3684(3)	.6229(5)	58(2)	69(3)	50(2)	-29(2)	32(2)	-21(2)
1	1.008(2)	-.116(1)	.194(2)	69(10)	74(10)	65(9)	-39(8)	41(8)	-28(7)
2	.926(2)	-.158(1)	.352(2)	67(9)	61(9)	68(9)	-29(7)	35(8)	-16(7)
3	.720(2)	-.117(1)	.208(2)	74(10)	75(10)	76(10)	-46(9)	37(8)	-28(8)
4	.626(2)	-.003(1)	.309(2)	79(11)	73(11)	92(12)	-34(9)	52(10)	-6(9)
5	.587(2)	.106(1)	.148(2)	62(10)	83(11)	69(10)	-27(8)	24(8)	8(8)
6	.739(2)	.155(1)	.266(2)	67(9)	47(8)	81(10)	-22(7)	39(8)	-8(7)
7	.875(2)	.111(1)	.136(2)	71(10)	70(10)	65(9)	-35(8)	38(8)	-1(7)
8	1.038(1)	-.000(1)	.288(2)	51(8)	70(9)	66(9)	-32(7)	26(7)	-13(7)
9	.714(2)	.348(1)	.603(2)	70(10)	89(11)	44(8)	-35(9)	20(7)	-19(7)
10	.561(1)	.416(1)	.691(2)	55(8)	79(10)	55(8)	-27(8)	17(7)	-2(7)
11	.603(1)	.354(1)	.935(2)	60(9)	96(12)	51(8)	-44(8)	22(7)	2(7)
12	.683(2)	.427(1)	1.127(2)	68(10)	96(12)	62(9)	-28(9)	40(8)	-26(8)
13	.888(2)	.360(1)	1.229(2)	66(10)	94(12)	44(8)	-34(9)	11(7)	-0(7)
14	.971(2)	.420(1)	1.106(2)	67(10)	80(11)	66(9)	-42(8)	26(8)	-22(8)
15	1.002(1)	.348(1)	.899(2)	54(8)	89(11)	53(8)	-27(8)	30(7)	-17(7)
16	.848(2)	.412(1)	.668(2)	72(10)	79(10)	59(9)	-25(8)	33(8)	11(7)

membered rings with distances of 3.80–3.95 Å and marked deviations from linearity (see Table 4). In $2S_8 \cdot SnI_4$ there are two crystallographically different iodine atoms having five and four sulfur atoms, respectively, as next neighbours. In the sulfur–selenium adduct there are four independent iodine atoms. I1 has contacts to two atoms from the ring molecules, I2 to five, I3 to four, and I4 to one atom. In both compounds all these distances are very near to the sums of van der Waals radii for iodine and sulfur or iodine and selenium and therefore all interactions between the eight-

membered rings and tin tetraiodide molecules must be considered to be very weak.

The intermolecular distances <4 Å are listed in Table 5. The shortest distances between the ring molecules are 3.42(6) and 3.40(3) Å for the sulfur and sulfur–selenium adducts, respectively. These distances are comparable to the intermolecular distances in eight-membered sulfur and selenium allotropes.^{16–21} The SnI_4 units are separated fairly widely in both adducts. In $2S_8 \cdot SnI_4$ each tetrahedron is surrounded by four other tin tetraiodide molecules with an $Sn \cdots Sn$ distance

Table 3. The bond lengths (Å) and angles (°) in $2S_8 \cdot SnI_4$ and $2S_n \cdot Se_{8-n} \cdot SnI_4$.

A. $2S_8 \cdot SnI_4$			
Sn1 - I1	2.659(10)	I1 - Sn1 - I2	107.6(3)
Sn1 - I2	2.666(10)	I1 - Sn1 - I1'	112.3(3)
		I1 - Sn1 - I2'	109.3(3)
		I2 - Sn1 - I2'	110.6(3)
S1 - S2	2.06(6)	S8 - S1 - S2	107(3)
S2 - S3	2.07(6)	S1 - S2 - S3	106(3)
S3 - S4	2.01(6)	S2 - S3 - S4	108(3)
S4 - S5	2.09(7)	S3 - S4 - S5	108(3)
S5 - S6	2.06(7)	S4 - S5 - S6	107(3)
S6 - S7	2.04(6)	S5 - S6 - S7	108(3)
S7 - S8	2.05(6)	S6 - S7 - S8	107(3)
S8 - S1	2.05(6)	S7 - S8 - S1	106(3)
B. $2S_n \cdot Se_{8-n} \cdot SnI_4$			
Sn1 - I1	2.654(7)	I1 - Sn1 - I2	111.7(2)
Sn1 - I2	2.682(5)	I1 - Sn1 - I3	107.7(2)
Sn1 - I3	2.669(7)	I1 - Sn1 - I4	111.3(2)
Sn1 - I4	2.673(6)	I2 - Sn1 - I3	106.9(2)
		I2 - Sn1 - I4	107.7(2)
		I3 - Sn1 - I4	111.4(2)
1 - 2	2.08(3)	8 - 1 - 2	107(1)
2 - 3	2.09(2)	1 - 2 - 3	106(1)
3 - 4	2.07(2)	2 - 3 - 4	107(1)
4 - 5	2.05(3)	3 - 4 - 5	108(1)
5 - 6	2.08(3)	4 - 5 - 6	107(1)
6 - 7	2.07(3)	5 - 6 - 7	108(1)
7 - 8	2.10(2)	6 - 7 - 8	108(1)
8 - 1	2.08(2)	7 - 8 - 1	109(1)
9 - 10	2.05(2)	16 - 9 - 10	108(1)
10 - 11	2.07(2)	9 - 10 - 11	108(1)
11 - 12	2.08(2)	10 - 11 - 12	107(1)
12 - 13	2.05(2)	11 - 12 - 13	107(1)
13 - 14	2.06(3)	12 - 13 - 14	107(1)
14 - 15	2.06(2)	13 - 14 - 15	108(1)
15 - 16	2.06(2)	14 - 15 - 16	108(1)
16 - 9	2.05(3)	15 - 16 - 9	108(1)

of 8.07 Å. In the sulfur-selenium adduct there are only three neighbouring tetrahedra with Sn...Sn distances from 7.82 to 8.10 Å. The shortest Sn...Sn distance in pure tin tetraiodide is 5.31 Å as calculated from the lattice and atomic parameters reported by Meller and Fankuchen.¹⁵ In $2S_8 \cdot SnI_4$ each SnI_4 unit is surrounded by twelve S_8 molecules and consequently each ring by six SnI_4 tetrahedra. In the sulfur-selenium adduct the packing is more complicated. There are two independent sulfur-selenium molecules. One is surrounded by six SnI_4 tetrahedra and the other

by four so that there are ten ring molecules around each tetrahedron. The unit cells as completed to show full molecules are presented in Fig. 1 for $2S_8 \cdot SnI_4$ and in Fig. 2 for $2S_n \cdot Se_{8-n} \cdot SnI_4$.

The wave numbers of the Raman lines of S_8 , SnI_4 and the two adducts are shown in Table 6. By comparing the spectrum of $2S_8 \cdot SnI_4$ to the spectra of the pure constituents it can be seen that adduct formation has very little effect on effect on the respective Raman lines which further demonstrates the weakness of the sulfur-iodine interaction. In the SS stretching region (480-

Table 4. Bond distances (Å) and angles (°) originating from iodine atoms.^a

A. 2S₈SnI₄			
I1–S1'	3.95(5)	Sn1–I1–S1'	85.7(8)
I1–S2	3.89(5)	Sn1–I1–S2	141.1(8)
I1–S7'	3.90(5)	Sn1–I1–S7'	140.3(8)
I1–S7'	3.95(5)	Sn1–I1–S7'	85.9(7)
I1–S8'	3.90(5)	Sn1–I1–S8'	74.7(6)
I2–S3'	3.87(5)	Sn1–I2–S3'	86.5(7)
I2–S3'	3.88(4)	Sn1–I2–S3'	144.6(8)
I2–S5'	3.97(5)	Sn1–I2–S5'	88.2(7)
I2–S6'	3.88(4)	Sn1–I2–S6'	146.9(8)
B. 2S_nSe_{8-n}SnI₄			
I1–5	3.95(2)	Sn1–I1–5	77.5(3)
I1–11'	3.86(2)	Sn1–I1–11'	144.5(3)
I2–4	3.81(2)	Sn1–I2–4	89.0(3)
I2–7'	3.93(1)	Sn1–2–7'	149.0(3)
I2–8'	3.95(2)	Sn1–I2–8'	144.0(3)
I2–9	3.97(2)	Sn1–I2–9	85.1(2)
I2–11	3.82(2)	Sn1–I2–11	88.6(2)
I3–1'	3.92(2)	Sn1–I3–1'	145.0(3)
I3–4'	3.79(2)	Sn1–I3–4'	89.1(3)
I3–8'	3.87(2)	Sn1–I3–8'	146.6(3)
I3–15'	3.84(2)	Sn1–I3–15'	87.9(3)
I4–15'	3.94(2)	Sn1–I4–15'	135.9(3)

^a Atoms denoted with ' have been generated from the parent atoms given in Table 2 by various symmetry operations.

Table 5. Intermolecular distances < 4 Å between the eight-membered rings.^a

A. 2S₈SnI₄			
S1–S1'	3.99(5)	S2–S6'	3.64(6)
S1–S6'	3.90(7)	S2–S7'	3.73(7)
S1–S7'	3.77(7)	S3–S5'	3.71(7)
S2–S5'	3.93(7)	S4–S8'	3.42(6)
B. 2S_nSe_{8-n}SnI₄			
1–7'	3.40(3)	8–8'	3.83(3)
1–9'	3.89(2)	9–12'	3.96(3)
1–15'	3.82(3)	10–10'	3.73(2)
2–6'	4.00(2)	10–12'	3.71(2)
2–8'	3.80(2)	11–12'	3.75(2)
2–15'	3.61(2)	12–12'	3.81(2)
3–5'	3.62(2)	13–16'	3.77(2)
6–8'	3.93(2)	14–14'	3.52(3)
6–11'	3.75(2)	14–15'	3.87(3)
7–11'	3.98(2)	14–16'	3.99(3)

^a Atoms denoted with ' have been generated from the parent atoms given in Table 2 by various symmetry operations.

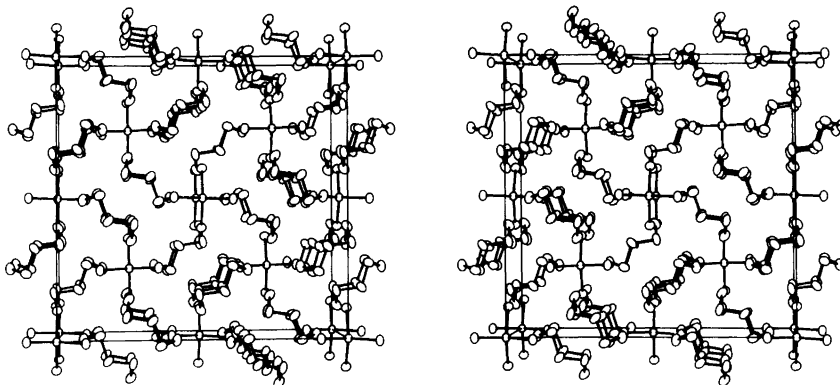


Fig. 1. Unit cell of $2S_8.SnI_4$ seen along c . The structure has been completed to show full molecules. a -Axis is vertical, b -axis horizontal.

429 cm^{-1}) additional lines are observed possibly due to splitting of the e_3 fundamental and activation of the b_1 fundamental as a consequence of the site symmetry C_1 . The general features of the SSS deformation region are the same in S_8 and the adduct but this region also shows the Raman lines of SnI_4 and the overlap apparently causes small differences in the positions and intensities. The region of torsional and lattice vibrations ($<100\text{ cm}^{-1}$) differs most, as expected.

The Raman spectrum of the sulfur–selenium adduct can be used to study the composition of this compound. Hawes¹¹ claimed that his adduct was either pure stoichiometric $2S_7Se.SnI_4$ or a mixture containing S_8 and S_7Se molecules depending on the conditions of the preparation. By comparing the Raman spectrum of the adduct to the spectra of the S_nSe_{8-n} phases reported earlier⁷ the following inferences can be made. Disregarding the Raman lines caused by tin

tetraiodide the spectrum of the sulfur–selenium adduct is strikingly similar to the spectra of the S_nSe_{8-n} phases. In the SSe stretching region ($390-290\text{ cm}^{-1}$) there are four lines indicating the presence of more than two SSe bonds and thus ruling out S_7Se as the only possible species. The narrow range of the observed SSe stretching vibrations which is comparable to the range observed in the sulfur–selenium phases, as well as the appearance of a Raman line at 265 cm^{-1} typical for SeSe stretching vibrations, indicate the presence of at least one selenium–selenium bond in the ring molecules of the adduct. In light of the similarity of the Raman spectra of the adduct and the sulfur–selenium phases it seems plausible that the adduct also contains different S_nSe_{8-n} rings present in varying concentrations, and with molecules containing selenium–selenium bonds being more abundant. However, a very weak Raman line at 296 cm^{-1} which is exceptionally

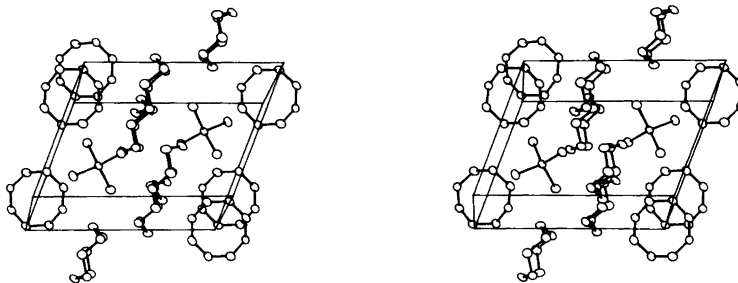


Fig. 2. Unit cell of $2S_nSe_{8-n}.SnI_4$ seen along c . The structure has been completed to show full molecules. a -Axis is vertical, b -axis horizontal.

Table 6. Raman spectra of S_8 , SnI_4 , $2S_8 \cdot SnI_4$, and $2S_n Se_{8-n} \cdot SnI_4$.

S_8 ²²	SnI_4	$2S_8 \cdot SnI_4$	$2S_n Se_{8-n} \cdot SnI_4$
473 vs		474 m	476 m-s 469 m
439 vw		445 vw 440 vw 430 vw	442 w 429 vw 382 m 364 w 348 w 296 vw 265 w
249 vw 245.5 vw		247 vw	248 vw 243 vw
218.5 vs 214 sh	216 w	216 s 212 sh	221 s 214 s 207 m 200 m
	209 w		194 sh 166 vw 157 m
187 vw		192 vw	147 vvs 137 w 128 vw 119 vw
153 s	147 vvs	160 w 149 vvs	92 w 83 w 78 sh 64 s
82.5 w		95 sh 84 m 72 sh	60 m 51 m
	65 s	68 s	47 m
62 vw 50 s	53 m	60 m 53 s	41 vw 34 w 30 m
42.5 m	39 vw	41 vw	27 m 22 m 16 s
		32 m	
27 w	28 w 24 w		

low in the SSe stretching region shows that there may also be sulfur–selenium rings with isolated selenium atoms in the adduct. The strong lines at 221 and 214 cm^{-1} presumably indicate the presence of S_8 in the adduct.

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