

Tetra- $\mu_2$ -selenido-diselenidobis[tris(2-aminoethyl)amine]dimanganese(II)ditin(IV)

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## Key indicators

Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.015$  Å  
 $R$  factor = 0.044  
 $wR$  factor = 0.111  
Data-to-parameter ratio = 18.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The centrosymmetric title compound,  $[\text{Mn}_2\text{Sn}_2\text{Se}_6(\text{C}_6\text{H}_{18}\text{N}_4)_2]$ , contains a central ditetrahedral edge-bridged  $[\text{Sn}_2\text{Se}_6]^{4-}$  anion, which connects two  $[\text{Mn}(\text{tren})]^{2+}$  fragments [tren is tris(2-aminoethyl)amine] through Mn–Se bonds of length 2.608 (2) Å to symmetry-related terminal Se atoms. These Se atoms also participate in additional weak Mn–Se interactions of length 3.122 (2) Å to the Mn atoms of symmetry-related  $[\text{Mn}(\text{tren})]^{2+}$  fragments, leading to the formation of infinite chains.

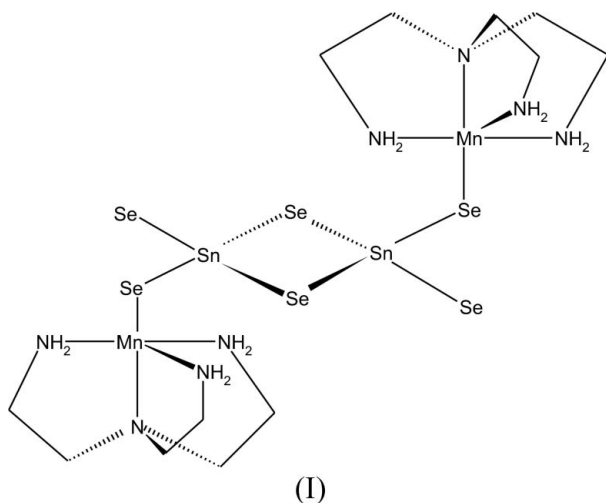
## Comment

Tetrahedral  $[\text{Sn}E_4]^{4-}$  ( $E$  is S, Se or Te) anions exhibit a characteristic tendency to condense in polar solvents to generate corner- or edge-bridged oligomeric or polymeric chalcogenidostannates(IV) (Sheldrick & Wachhold, 1998; Sheldrick, 2000). Ditetrahedral  $[\text{Sn}_2E_6]^{4-}$  anions containing two edge-sharing tetrahedra are particularly common and have been structurally characterized for  $E = \text{Se}$  in many salts, for instance in the alkali metal hexaselenidostannates(IV),  $\text{Na}_4\text{Sn}_2\text{Se}_6 \cdot 13\text{H}_2\text{O}$  (Krebs & Uhlen, 1987) and  $M_4\text{Sn}_2\text{Se}_6$  ( $M$  is K, Rb or Cs) (Eisenmann & Hansa, 1993; Sheldrick & Schaaf, 1994; Sheldrick & Braunbeck, 1989). Selenidostannate(IV) anions are potential terminal or bridging ligands and have been employed to construct polymeric ternary anions, as in the quaternary phases  $\text{K}_2\text{MnSnSe}_4$ ,  $\text{K}_2\text{MnSn}_2\text{Se}_6$  and  $\text{K}_2\text{Ag}_2\text{SnSe}_4$  (Chen *et al.*, 2000),  $\text{K}_2\text{Ag}_2\text{Sn}_2\text{Se}_6$  (Guo *et al.*, 2001),  $\text{Na}_3\text{CuSnSe}_4$  (Klepp & Fabian, 1997), and  $\text{K}_2\text{Au}_2\text{Sn}_2\text{Se}_6$  (Loeken & Tremel, 1998). Behrens *et al.* (2003) have also recently demonstrated that  $\text{Co}^{\text{II}}$  and  $\text{Ni}^{\text{II}}$  atoms can be incorporated into the thiostannates(IV),  $[\{\text{Co}(\text{tren})\}_2(\mu\text{-Sn}_2\text{S}_6)]$  and  $[\{\text{Ni}(\text{tren})\}_2(\mu\text{-Sn}_2\text{S}_6)]$ , in which four of the transition metal coordination sites are occupied by the N-donor atoms of tris(2-aminoethyl)amine (tren). This finding prompted us to investigate whether the  $[\text{Sn}_2\text{Se}_6]^{4-}$  anion can likewise be employed to prepare analogous transition metal selenidostannates and we now report the solvothermal preparation and structure of the title compound,  $[\{\text{Mn}(\text{tren})\}_2(\mu\text{-Sn}_2\text{Se}_6)]$ , (I).

Compound (I) (Fig. 1) contains a centrosymmetric  $[\text{Sn}_2\text{Se}_6]^{4-}$  anion, whose symmetry-related terminal Se2 atoms coordinate the Mn atoms of  $[\text{Mn}(\text{tren})]^{2+}$  fragments. As typically observed for  $[\text{Sn}_2\text{Se}_6]^{4-}$  anions (Sheldrick & Braunbeck, 1993), the more polar terminal Sn1–Se2 and Sn1–Se3 distances of 2.488 (1) and 2.447 (1) Å are significantly shorter than the bridging Sn1–Se1 distances of 2.583 (2) and 2.592 (1) Å. The lengthening of Sn1–Se2 relative to Sn1–Se3 is due to its participation in an Se2–Mn1 bond of length 2.608 (2) Å. This Se atom also completes the octahedral coordination environment of a symmetry-related Mn1 atom at

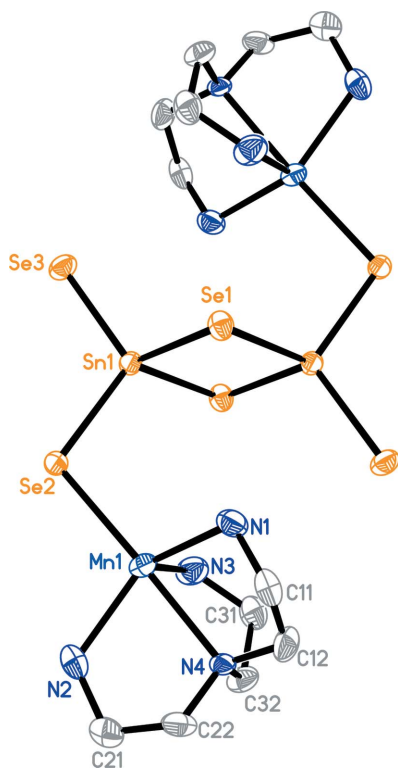
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$(-x, -y, 2 - z)$  through a weak  $\text{Se}2 \cdots \text{Mn}1$  interaction [3.122 (2) Å]. As a result, individual  $[\{\text{Mn}(\text{tren})\}_2(\mu\text{-Sn}_2\text{Se}_6)]$  units are linked into infinite chains. It is interesting to note that, although not isomorphous with (I), the monoclinic compound  $[\{\text{Ni}(\text{tren})\}_2(\mu\text{-Sn}_2\text{S}_6)]$  (Behrens *et al.*, 2003) also adopts a similar connectivity pattern.

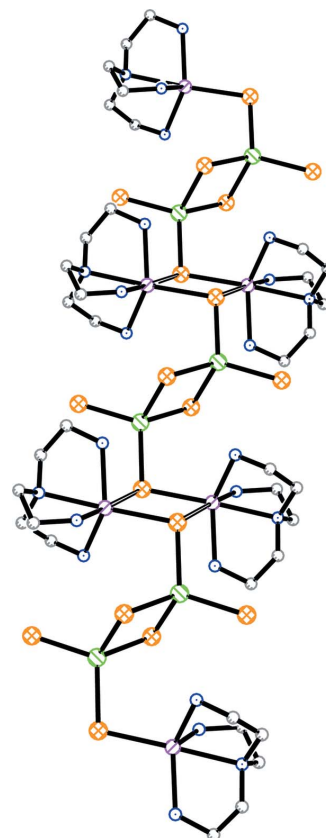


### Experimental

$\text{SnSe}$  (103.6 mg, 0.52 mmol) and  $[\text{MnCl}_2(\text{tren})]$  (138.5 mg 0.50 mmol) were heated to 463 K in a 1:1 mixture (1 ml) of  $\text{CH}_3\text{OH}$  and  $\text{H}_2\text{O}$  in



**Figure 1**  
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. Unlabelled atoms are generated by the symmetry operator  $(1 - x, 1 - y, 2 - z)$ .



**Figure 2**  
The infinite chains of (I) resulting from additional weak  $\text{Se}2 \cdots \text{Mn}1$  interactions. H atoms have been omitted.

the presence of  $\text{Cs}_2\text{CO}_3$  (165.9 mg, 0.51 mmol). After 30 h, the solution was cooled to 293 K at a rate of  $1.5 \text{ K h}^{-1}$  to afford yellow crystals of  $[\{\text{Mn}(\text{tren})\}_2(\mu\text{-Sn}_2\text{Se}_6)]$ , (I), in 43% yield.

### Crystal data

$[\text{Mn}_2\text{Sn}_2\text{Se}_6(\text{C}_6\text{H}_{18}\text{N}_4)_2]$   
 $M_r = 1113.51$   
 Triclinic,  $P\bar{1}$   
 $a = 7.772$  (3) Å  
 $b = 8.193$  (3) Å  
 $c = 12.481$  (4) Å  
 $\alpha = 97.36$  (4)°  
 $\beta = 104.432$  (18)°  
 $\gamma = 107.26$  (3)°

$V = 717.2$  (4) Å<sup>3</sup>  
 $Z = 1$   
 $D_x = 2.578 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 10.21 \text{ mm}^{-1}$   
 $T = 292$  (2) K  
 Prism, yellow  
 $0.54 \times 0.11 \times 0.10 \text{ mm}$

### Data collection

Siemens P4 four-circle diffractometer  
 $\omega$  scans  
 Absorption correction:  $\psi$  scan (*XPRED* in *SHELXTL*; Sheldrick, 1995)  
 $T_{\min} = 0.272$ ,  $T_{\max} = 0.363$   
 3093 measured reflections

2497 independent reflections  
 1869 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.053$   
 $\theta_{\max} = 25.0^\circ$   
 3 standard reflections every 100 reflections  
 intensity decay: 2.7%

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.111$   
 $S = 1.02$   
 2497 reflections  
 136 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0592P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 1.52 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -1.16 \text{ e \AA}^{-3}$

**Table 1**Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots Se3^i$	0.90	2.76	3.636 (8)	165
$N3-H3B\cdots Se1^i$	0.90	2.74	3.634 (8)	173
$N1-H1B\cdots Se1^{ii}$	0.90	3.03	3.790 (8)	144
$N2-H2A\cdots Se1^{iii}$	0.90	2.86	3.708 (8)	157
$N2-H2B\cdots Se3^{iv}$	0.90	2.74	3.561 (8)	153
$N3-H3A\cdots Se3^{iv}$	0.90	3.02	3.829 (9)	151

Symmetry codes: (i)  $-x+1, -y+1, -z+2$ ; (ii)  $-x, -y+1, -z+2$ ; (iii)  $-x, -y, -z+2$ ; (iv)  $-x+1, -y, -z+2$ .

H atoms were constrained to idealized positions and refined using a riding model, with  $C-H = 0.97$  and  $N-H = 0.90$   $\text{\AA}$ , and with  $U_{iso}(H) = 1.2U_{eq}(C)$  or  $1.2U_{eq}(N)$ . The highest peak is located 1.14  $\text{\AA}$  from atom Sn1 and the deepest hole 0.98  $\text{\AA}$  from atom Sn1.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXTL*.

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