

Acta Crystallographica Section C

**Crystal Structure
Communications**

ISSN 0108-2701

***trans*-Bis[ethane-1,2-dithiolato(2-)-*S,S'*]bis(2-mercaptopyridine-*S*)tin(IV)**

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Electronic paper

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trans-Bis[ethane-1,2-dithiolato(2-)-*S,S'*]bis(2-mercaptopyridine-*S*)tin(IV)

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Received 20 July 2000

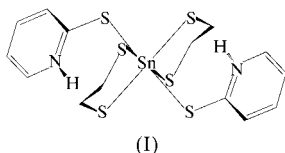
Accepted 8 August 2000

Data validation number: IUC0000210

The title compound, $[\text{Sn}(\text{C}_3\text{H}_5\text{NS})_2(\text{C}_2\text{H}_4\text{S}_2)_2]$, was obtained from a 1:2 mixture of bis(ethane-1,2-dithiolato)tin(IV) and 2-mercaptopyridine. The molecules are discrete monomeric *trans*-octahedral units, with the Sn^{IV} atom at the centre of symmetry, planar 2-mercaptopyridine zwitterions and SnS_2C_2 groups in twist-envelope conformations. The 2-mercaptopyridine ligands are monodentate and are bonded through the S atoms. The S—Sn distances between the S atom of edt (edt is ethane-1,2-dithiolate) and the Sn atom are 2.473 (1) and 2.505 (1) Å, which are slightly longer than the S—Sn distance in $\text{Sn}(\text{edt})_2$ of 2.390 (1) Å. The bond between the 2-mercaptopyridine S atom and the Sn atom are, remarkably, weaker than the S—Sn bond involving edt.

Comment

This is the first X-ray crystallographic study of bis(ethane-1,2-dithiolato)tin(IV) bearing two 2-mercaptopyridine ligands, (I). Research on the coordination of $[\text{Sn}(\text{C}_2\text{H}_4\text{S}_2)_2]$ with ligands contained N or S is important for realising the coordination characteristics of the Sn atom. Up until now, some compounds of this type were reported, e.g. $[\text{Sn}(\text{edt})_2(\text{C}_3\text{H}_5\text{N}_3)_2]$ (Bandoli *et al.*, 1993a), $[\text{Sn}(\text{edt})_2(\text{SCH}_3)]^-$ (Krebs *et al.*, 1986) and $[\text{Sn}_2(\text{edt})_5]^{2-}$ (Holmes *et al.*, 1988).



Experimental

$\text{Sn}(\text{edt})_2$ (0.303 g, 1 mmol), prepared according to the literature method of Bandoli *et al.* (1993b), and 2-mercaptopyridine (0.222 g,

2 mmol), purchased from Arcos, were dissolved in dichloromethane and the solution stirred. The solvent was left to evaporate slowly at room temperature. After 3 d, the pale-yellow crystals which had formed were filtered off.

Crystal data

$[\text{Sn}(\text{C}_3\text{H}_5\text{NS})_2(\text{C}_2\text{H}_4\text{S}_2)_2]$
 $M_r = 525.35$
 Monoclinic, $P2_1/c$
 $a = 7.162$ (2) Å
 $b = 15.101$ (4) Å
 $c = 9.035$ (4) Å
 $\beta = 96.89$ (2)°
 $V = 970.2$ (6) Å³
 $Z = 2$

$D_x = 1.798$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 3872 reflections
 $\theta = 2.64$ – 25.03 °
 $\mu = 1.961$ mm⁻¹
 $T = 293$ (2) K
 Hexagonal, pale yellow
 $0.38 \times 0.30 \times 0.08$ mm

Data collection

Siemens SMART CCD diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.572$, $T_{\text{max}} = 0.890$
 4953 measured reflections

1716 independent reflections
 1517 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.0254$
 $\theta_{\text{max}} = 25.03$ °
 $h = -8 \rightarrow 6$
 $k = -17 \rightarrow 15$
 $l = -9 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.084$
 $S = 1.061$
 1716 reflections
 125 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 1.6585P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.76$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.59$ e Å⁻³

There was positional disorder of one of the two equatorial C atoms of edt over two sites (C21 and C211), both of which formed a five-membered ring with two S atoms of edt and the Sn atom. The population of these disordered atoms were assumed to be 0.6 and 0.4. The H atoms of 2-mercaptopyridine were included in the structure calculation. The H atoms of C21 and C31 were omitted because of the disorder of the C21 atom.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1994); data reduction: SMART (Siemens, 1996); program(s) used to solve structure: SHELXTL (Siemens, 1994); program(s) used to refine structure: SHELXTL.

This research was supported by grants from the State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, and the CNSF, CAS and Fujian province.

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