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Silver(I) *o*-Nitrobenzoate

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Abstract

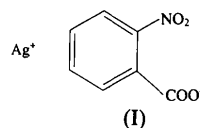
The title compound, [Ag(C₇H₄NO₄)], was obtained from silver nitrate and 2-nitrobenzoic acid in aqueous solution. The crystal comprises a three-dimensional polymeric network with short Ag—Ag distances [2.804 (1) and 2.892 (1) Å]. All three Ag atoms of the asymmetric unit are included in eight-membered rings (Ag—O—C—O)₂ with two types of coordination: (a) a trigonal bipyramidal arrangement (for one Ag atom of the asymmetric unit), the Ag atom being linked to another Ag atom [Ag—Ag 2.804 (1) Å] and to four O atoms [Ag—O 2.257 (6), 2.247 (5), 2.414 (4), 2.533 (5) Å], and (b) a tetrahedral arrangement (for two Ag atoms of the asymmetric unit), where each Ag atom is linked to another [Ag—Ag 2.892 (1) Å] and to three O atoms [Ag—O 2.167 (6), 2.210 (6), 2.456 (5) Å for one atom, Ag—O 2.125 (6), 2.182 (5), 2.506 (4) Å for the other]. Moreover, the *o*-nitrobenzoato ligands show three different conformations induced by the coordination modes, with rotations of the NO₂ and CO₂ groups, resulting in all the atoms of each ligand not being located in the same plane.

Comment

Except for that of silver(I) *p*-aminobenzoate (Amiraslanov, Usabaliev, Nadzhafov, Musaev, Movsumov & Mamedov, 1980), all the reported silver(I) monocarboxylate crystal structures show only one coordination type for the metal; a further exception is the structure of silver(I) malonate, AgCO₂CH₂CO₂Ag, in which there are two very different types of silver(I) coordination (Charbonnier, Faure & Loiseleur, 1981).

As a part of our work on the coordination modes of silver(I) in different carboxylates (Charbonnier,

Faure & Petit-Ramel, 1992), we report here a surprising new structure with three silver coordination environments. All three Ag atoms in the asymmetric



unit of the title compound (I), Ag1, Ag2 and Ag3, are included in eight-membered rings, (Ag—O—C—O)₂, but there are two types of coordination. In the first, Ag1 is surrounded by one other Ag1 atom [Ag1—Ag1ⁱ 2.804 (1) Å] and by four O atoms [Ag1—O12ⁱ 2.257 (6), Ag1—O11 2.247 (5), Ag1—O32ⁱⁱ 2.414 (4), Ag1—O31 2.533 (5) Å], forming a trigonal bipyramid (Fig. 1). The short Ag1—Ag1ⁱ distance is very close to the values found in some other carboxylates: 2.809 (1) Å (Mak, Yip, Kennard, Smith & O'Reilly, 1988), 2.814 (2) Å (Chen & Mak, 1991). In the second type of coordination, Ag2 and Ag3, belonging to similarly distorted tetrahedra, are each coordinated by one Ag atom [Ag2ⁱⁱⁱ—Ag3 2.892 (1) Å] and by three O atoms [Ag2ⁱⁱⁱ—O21 2.167 (6), Ag2ⁱⁱⁱ—O32 2.210 (6), Ag2ⁱⁱⁱ—O12ⁱⁱⁱ 2.456 (3) Å; Ag3—O22 2.125 (6), Ag3—O31 2.182 (5), Ag3—O11 2.506 (4) Å] (Fig. 1). The distance Ag2ⁱⁱⁱ—Ag3 is longer than Ag1—Ag1ⁱ and is very close to those found in other silver(I) carboxylates: 2.856 (2) Å (Huang, Lü, Chen & Mak, 1991), 2.881 (2) Å (Charbonnier, Faure, Petit-Ramel & Loiseleur, 1984), 2.898 (1) Å (Chen & Mak, 1991). The Ag—O distances are within the range of values reported for other carboxylates (Huang *et al.*, 1991;

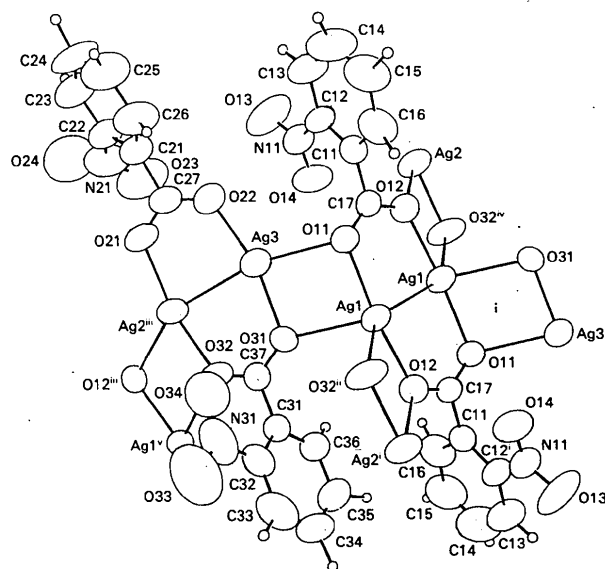


Fig. 1. Coordination environment of the silver atoms. Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (iv) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (v) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$.

Chen & Mak, 1991; Mak *et al.*, 1988; Amiraslanov *et al.*, 1980; Hedrich & Hartl, 1983; Charbonnier *et al.*, 1984).

The crystal structure of silver(I) *o*-nitrobenzoate is a three-dimensional polymeric network of eight-membered and four-membered rings (Fig. 2). The involvement of Ag atoms in such rings has already been observed in other carboxylates (Huang *et al.*, 1991; Chen & Mak, 1991; Mak *et al.*, 1988; Amiraslanov *et al.*, 1980; Hedrich & Hartl, 1983; Charbonnier *et al.*, 1984). In the eight-membered rings, the values of the O—Ag—O angles [O11—Ag1—O12ⁱ 163.3 (1), O22—Ag3—O31 163.6 (1)°] and the O—Ag—Ag angles [O11—Ag1—Ag1ⁱ 83.7 (1)°, O22—Ag3—Ag2ⁱⁱⁱ 81.5 (1)°] are in good agreement with the values determined previously for analogous structures (Mak *et al.*, 1988; Chen & Mak, 1991; Huang *et al.*, 1991).

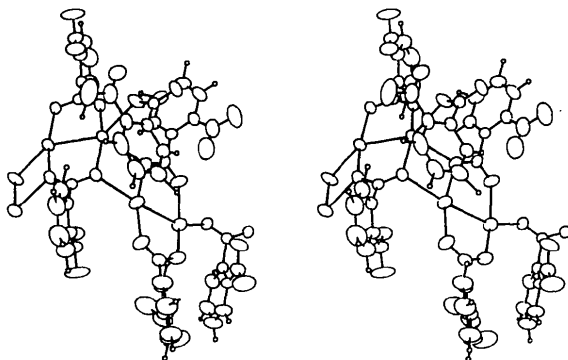


Fig. 2. Stereoview of the title compound.

In this structure the *o*-nitrobenzoate ligand presents three different conformations. The O atoms of the CO₂ and NO₂ substituents are located out of the phenyl ring plane (denoted Ph). A twisted conformation is already known for the free ligand. Indeed, the crystal structure of 2-nitrobenzoic acid (Tavale & Pant, 1973) displays Ph/NO₂ and Ph/CO₂ dihedral angles of 54.1 and 24.1°, respectively; thus, the overcrowding between the two NO₂ and CO₂ substituents linked to the phenyl ring manifests itself as a twisting of the substituents from the phenyl plane. In the Ag compound these values are modified (Table 3). Nevertheless, Muhonen's proposition (1983) is verified: the sum of the two dihedral angles between the phenyl plane and each substituent plane is nearly 90°. According to Muhonen (1983), the magnitude of the dihedral angles depends on factors such as intermolecular contacts and coordination of the substituents. Table 3 shows that the dihedral angle between the CO₂ plane and the benzene ring is always greater than those between the ring and the

NO₂ plane. This fact can be explained by the importance of the size of the eight-membered ring. Therefore, the steric crowding between eight-membered and phenyl rings increases this torsion. The stabilization of these conformations is induced by the coordination bonds between the carboxylate groups and the Ag atoms.

Experimental

The silver(I) complex was prepared by dissolving equimolar amounts of 2-nitrobenzoic acid and silver(I) nitrate in water. A white precipitate was obtained by successive NaOH additions to pH 5. The dissolution of the precipitate in hot water gave a clear solution, which afforded colourless crystals by slow evaporation in the dark at room temperature.

Crystal data

[Ag(C₇H₄NO₄)]
 $M_r = 273.98$
 Monoclinic
 $C2/c$
 $a = 39.262 (4) \text{ \AA}$
 $b = 7.897 (1) \text{ \AA}$
 $c = 46.352 (5) \text{ \AA}$
 $\beta = 160.47 (2)^\circ$
 $V = 4804 (4) \text{ \AA}^3$
 $Z = 24$
 $D_x = 2.24 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 $\lambda = 0.7107 \text{ \AA}$
 Cell parameters from 25 reflections
 $\theta = 10.83\text{--}16.66^\circ$
 $\mu = 2.47 \text{ mm}^{-1}$
 $T = 291 \text{ K}$
 Flat
 $0.4 \times 0.4 \times 0.1 \text{ mm}$
 Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
 ω –5/3 θ scans
 Absorption correction: empirical
 $T_{\min} = 0.80$, $T_{\max} = 0.99$
 7946 measured reflections
 5766 independent reflections
 4399 observed reflections
 $[I > 3\sigma(I)]$

$\theta_{\max} = 27^\circ$
 $h = 0 \rightarrow 36$
 $k = 0 \rightarrow 10$
 $l = -51 \rightarrow 19$
 3 standard reflections
 frequency: 60 min
 intensity variation: 0.6%

Refinement

Refinement on F
 $R = 0.028$
 $wR = 0.046$
 $S = 2.65$
 4399 reflections
 352 parameters
 H-atom parameters not refined

$w = 1/\sigma^2(F_o)$
 $(\Delta/\sigma)_{\max} = 0.97$
 $\Delta\rho_{\max} = 0.53 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.58 \text{ e \AA}^{-3}$
 Extinction correction: none
 Atomic scattering factors from SDP (B. A. Frenz & Associates, Inc., 1982)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$)

	$B_{\text{eq}} = (4/3)\sum_i \sum_j \beta_{ij} a_i \cdot a_j$			
	<i>x</i>	<i>y</i>	<i>z</i>	B_{eq}
Ag1	0.42101 (1)	0.56587 (7)	0.41995 (1)	3.22 (1)
Ag2	0.81518 (1)	0.31042 (8)	0.73223 (1)	4.03 (1)
Ag3	0.44744 (1)	0.42123 (9)	0.36839 (1)	4.46 (1)
O11	0.5421 (1)	0.5792 (6)	0.48242 (9)	3.1 (1)
O12	0.6712 (1)	0.5086 (5)	0.61461 (9)	3.0 (1)

O21	0.4228 (1)	0.2462 (7)	0.2840 (1)	4.1 (1)
O22	0.5323 (1)	0.4016 (8)	0.3972 (1)	4.9 (1)
O31	0.3241 (1)	0.4287 (6)	0.3015 (1)	3.9 (1)
O32	0.2203 (1)	0.2616 (6)	0.1939 (1)	3.9 (1)
C11	0.7087 (2)	0.6357 (7)	0.5995 (1)	2.6 (1)
C12	0.7556 (2)	0.5497 (8)	0.6147 (1)	3.1 (2)
C13	0.8227 (2)	0.626 (1)	0.6494 (2)	4.8 (2)
C14	0.8451 (2)	0.796 (1)	0.6714 (2)	5.9 (2)
C15	0.8012 (2)	0.8880 (9)	0.6583 (2)	5.0 (2)
C16	0.7343 (2)	0.8080 (8)	0.6233 (2)	4.0 (2)
C17	0.6345 (2)	0.5640 (7)	0.5621 (1)	2.4 (1)
O13	0.7729 (1)	0.2965 (8)	0.6047 (1)	6.7 (2)
O14	0.6874 (1)	0.2966 (6)	0.5751 (1)	4.6 (1)
N11	0.7367 (1)	0.3689 (7)	0.5962 (1)	3.6 (1)
C21	0.5669 (2)	0.3589 (9)	0.3761 (2)	3.4 (2)
C22	0.5933 (2)	0.2314 (9)	0.3777 (2)	3.7 (2)
C23	0.6442 (2)	0.263 (1)	0.3929 (2)	5.0 (2)
C24	0.6705 (2)	0.433 (1)	0.4075 (2)	5.6 (2)
C25	0.6458 (2)	0.559 (1)	0.4065 (2)	5.6 (2)
C26	0.5947 (2)	0.522 (1)	0.3911 (2)	4.7 (2)
C27	0.5029 (2)	0.3319 (9)	0.3515 (1)	3.3 (2)
O23	0.5793 (2)	0.0071 (8)	0.3973 (1)	7.0 (2)
O24	0.5593 (2)	-0.0432 (9)	0.3366 (2)	8.5 (2)
N21	0.5738 (2)	0.0517 (8)	0.3685 (2)	5.1 (2)
C31	0.1540 (2)	0.4026 (7)	0.1817 (1)	2.6 (1)
C32	0.0719 (2)	0.5072 (8)	0.1097 (1)	3.2 (2)
C33	-0.0063 (2)	0.5334 (9)	0.0665 (2)	4.8 (2)
C34	-0.0044 (2)	0.459 (1)	0.0943 (2)	5.3 (2)
C35	0.0779 (2)	0.355 (1)	0.1680 (2)	5.0 (2)
C36	0.1561 (2)	0.3274 (9)	0.2106 (1)	3.4 (2)
C37	0.2394 (2)	0.3638 (7)	0.2294 (1)	2.6 (1)
O33	-0.0115 (2)	0.6712 (9)	0.0095 (2)	8.2 (2)
O34	0.1420 (2)	0.5973 (8)	0.1230 (1)	6.0 (2)
N31	0.0675 (2)	0.5985 (7)	0.0791 (1)	4.6 (2)

Table 2. Selected geometric parameters (Å, °)

Ag1—O11	2.247 (5)	C12—N11	1.458 (8)
Ag1—O31	2.533 (5)	C13—C14	1.39 (1)
Ag1—Ag1 ⁱ	2.804 (1)	C14—C15	1.38 (2)
Ag1—O12 ⁱ	2.257 (6)	C15—C16	1.38 (1)
Ag1—O32 ⁱⁱ	2.414 (4)	O13—N11	1.20 (1)
Ag2—O12	2.456 (3)	C34—C35	1.407 (8)
Ag3—O11	2.506 (4)	C35—C36	1.40 (1)
Ag3—O22	2.125 (6)	O33—N31	1.224 (5)
Ag3—O31	2.182 (5)	O14—N11	1.209 (9)
Ag3—Ag2 ⁱⁱⁱ	2.892 (1)	C21—C22	1.40 (1)
O11—C17	1.249 (2)	C21—C26	1.38 (1)
O12—C17	1.257 (8)	C21—C27	1.50 (1)
O21—C27	1.260 (5)	C22—C23	1.38 (1)
C32—C33	1.37 (1)	C22—N21	1.47 (1)
C32—N31	1.45 (1)	C23—C24	1.42 (1)
C33—C34	1.35 (2)	C24—C25	1.35 (1)
O21—Ag2 ⁱⁱⁱ	2.167 (6)	C25—C26	1.39 (2)
O22—C27	1.23 (1)	O23—N21	1.19 (1)
O31—C37	1.242 (3)	O24—N21	1.22 (1)
O32—C37	1.260 (9)	C31—C32	1.390 (5)
O32—Ag2 ⁱⁱⁱ	2.210 (6)	C31—C36	1.39 (1)
C11—C12	1.38 (1)	C31—C37	1.501 (9)
C11—C16	1.410 (8)	O34—N31	1.213 (9)
C11—C17	1.513 (9)	O12 ⁱⁱⁱ —Ag2 ⁱⁱⁱ	2.456 (3)
C12—C13	1.38 (1)		
O11—Ag1—O31	81.1 (1)	C12—N11—O14	118.4 (7)
O11—Ag1—Ag1 ⁱ	83.7 (1)	O13—N11—O14	122.5 (6)
O11—Ag1—O12 ⁱ	163.3 (1)	C22—C21—C26	117.0 (8)
O11—Ag1—O32 ⁱⁱ	119.9 (1)	C22—C21—C27	124.4 (6)
O31—Ag1—Ag1 ⁱ	129.4 (1)	C26—C21—C27	118.4 (7)
O31—Ag1—O12 ⁱ	102.9 (1)	C21—C22—C23	122.7 (7)
O31—Ag1—O32 ⁱⁱ	82.7 (9)	C21—C22—N21	121.4 (8)
Ag1 ⁱ —Ag1—O12 ⁱ	81.3 (1)	C23—C22—N21	115.7 (8)
Ag1 ⁱ —Ag1—O32 ⁱⁱ	144.7 (1)	C22—C23—C24	118.1 (9)
O12 ⁱ —Ag1—O32 ⁱⁱ	76.7 (1)	C23—C24—C25	120 (1)
O11—Ag3—O22	112.4 (1)	C24—C25—C26	120.7 (8)
O11—Ag3—O31	82.9 (1)	C21—C26—C25	121.6 (8)
O11—Ag3—Ag2 ⁱⁱⁱ	163.9 (1)	O21—C27—O22	127.4 (8)
O22—Ag3—O31	163.6 (1)	O21—C27—C21	116.0 (7)
O22—Ag3—Ag2 ⁱⁱⁱ	81.5 (1)	O22—C27—C21	116.6 (4)
O31—Ag3—Ag2 ⁱⁱⁱ	84.3 (1)	C22—N21—O23	117.8 (7)

Ag1—O11—Ag3	97.35 (8)	C22—N21—O24	117.6 (9)
Ag1—O11—C17	121.9 (5)	O23—N21—O24	124.4 (7)
Ag3—O11—C17	126.1 (4)	C32—C31—C36	117.4 (6)
Ag2—O12—C17	124.1 (4)	C32—C31—C37	124.5 (7)
Ag2—O12—Ag1 ⁱ	101.9 (2)	C36—C31—C37	118.1 (4)
C17—O12—Ag1 ⁱ	124.9 (2)	C31—C32—C33	122.2 (8)
C27—O21—Ag2 ⁱⁱⁱ	124.1 (6)	C31—C32—N31	120.6 (7)
Ag3—O22—C27	125.5 (3)	C33—C32—N31	117.2 (5)
Ag1—O31—Ag3	98.25 (7)	C32—C33—C34	120.3 (5)
Ag1—O31—C37	138.9 (5)	C33—C34—C35	120.2 (8)
Ag3—O31—C37	122.6 (5)	C34—C35—C36	118.8 (9)
C37—O32—Ag2 ⁱⁱⁱ	129.4 (3)	C31—C36—C35	121.1 (5)
C12—C11—C16	116.9 (7)	O31—C37—O32	124.7 (6)
C12—C11—C17	127.0 (5)	O31—C37—C31	118.4 (6)
C16—C11—C17	116.1 (7)	O32—C37—C31	116.9 (3)
C11—C12—C13	122.9 (6)	C32—N31—O33	118.8 (7)
C11—C12—N11	119.2 (6)	C32—N31—O34	118.6 (4)
C13—C12—N11	117.9 (7)	O33—N31—O34	122.6 (9)
C12—C13—C14	118.2 (9)	Ag1—Ag1 ⁱ —O12	81.27 (6)
C13—C14—C15	121.5 (9)	Ag3—Ag2 ⁱⁱⁱ —O21	80.6 (1)
C14—C15—C16	119.0 (7)	Ag3—Ag2 ⁱⁱⁱ —O32	77.92 (8)
C11—C16—C15	121.6 (8)	Ag3—Ag2 ⁱⁱⁱ —O12 ⁱⁱⁱ	152.8 (1)
O11—C17—O12	126.4 (6)	O21—Ag2 ⁱⁱⁱ —O32	152.5 (2)
O11—C17—C11	116.3 (6)	O21—Ag2 ⁱⁱⁱ —O12 ⁱⁱⁱ	126.4 (1)
O12—C17—C11	117.0 (2)	O32—Ag2 ⁱⁱⁱ —O12 ⁱⁱⁱ	76.7 (2)
C12—N11—O13	119.0 (6)		

Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iii) $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$.

Table 3. Dihedral angles (°)

Plane definitions: I (O11, O12, C17); II (C11, C12, C13, C14, C15, C16); III (O13, O14, N11); IV (C21, C22, C23, C24, C25, C26); V (O21, O22, C27); VI (C31, C32, C33, C34, C35, C36); VII (O23, O24, N21); VIII (O31, O32, C37); IX (O33, O34, N31).

Ph/CO ₂	Angle	Ph/NO ₂	Angle	CO ₂ /NO ₂	Angle
II [^] I	89.9 (3)	II [^] III	7.7 (8)	I [^] III	87.4 (4)
IV [^] V	49.0 (3)	IV [^] VII	33.8 (2)	V [^] VII	55.6 (7)
VI [^] VIII	105.6 (3)	VI [^] IX	10 (2)	VIII [^] IX	107.2 (5)

Program used: Enraf-Nonius *SDP* system (B. A. Frenz & Associates, Inc., 1982). Molecular graphics: *ORTEP* (Johnson, 1965). All calculations were performed on a DEC MicroVAX 3100-80 computer at the Centre de diffractométrie Automatique, Université Lyon I.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: DU1062). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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cis-Dichlorobis(*N,N*-diethyldithiocarbamato-*S,S'*)tin(IV)

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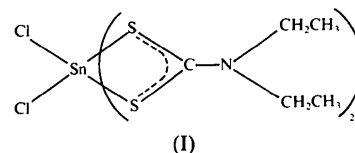
Abstract

The structural features of the title complex, $[\text{SnCl}_2(\text{C}_5\text{H}_{10}\text{NS}_2)_2]$, are significantly different to those of the complexes $\text{Me}_2\text{Sn}(\text{S}_2\text{CNR}_2)_2$ that have been structurally characterized so far. In the title complex the geometry around the Sn atom is *cis*-octahedral with a Cl—Sn—Cl angle of $91.85(3)^\circ$ and an average Sn—Cl bond length of $2.404(7) \text{ \AA}$. Both dithiocarbamato groups behave as bidentate chelating ligands with an average Sn—S bond length of $2.539(6) \text{ \AA}$ and an average S—Sn—S bond angle of $71.01(2)^\circ$.

Comment

Crystallographic studies of dithiocarbamato complexes of diorganotin(IV) species $\text{R}_2\text{Sn}(\text{S}_2\text{CNR}_2)_2$ have revealed a variety of coordination geometries about the Sn atom, ranging from tetrahedral to distorted octahedral, as well as dithiocarbamato ligands that are either bidentate or monodentate (Fuzue, Kimura, Yasuoka, Kasai & Kakudo, 1970; Kimura, Yasuoka, Kasai & Kakudo, 1972; Sheldrick & Sheldrick, 1970). In the crystal structure of $[(\text{Et}_2\text{NCS}_2)_2\text{Sn}\{\text{O}=\text{C}(\text{CH}_3)=\text{C}(\text{S})-\text{C}(\text{O})-\text{CH}_3\}]$, a novel mixed-ligand complex of tin(IV) (Sharma, Bohra & Mehrotra, 1993), both dithiocarbamato ligands are essentially bidentate [average Sn—S bond length $2.547(4) \text{ \AA}$].

The metal environment in the title compound $[\text{Cl}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2]$, (I), differs from that in $\text{Me}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$ (Lockhart, Manders, Schlemper & Zuckerman, 1986) in having methyl groups replaced by more electronegative chloro groups. This results



in a significant change in coordination geometry from distorted *trans*-octahedral in $\text{Me}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$ to *cis*-octahedral in $\text{Cl}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$. The structural features of $\text{Cl}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$ are also significantly different from those of the dimethyltin bis(dithiocarbamates) $\text{Me}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$ (Lockhart *et al.*, 1986), $\text{Me}_2\text{Sn}\{\text{S}_2\text{CN}(\text{CH}_2)_4\}_2$ (Lockhart, Manders & Schlemper, 1985) and $\text{Me}_2\text{Sn}(\text{S}_2\text{CNMe}_2)_2$ (Kimura *et al.*, 1972) that have been structurally characterized so far. The dithiocarbamato ligands in $\text{Me}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$ are bidentate, chelating to Sn with one long and one short Sn—S bond [average lengths $2.996(3)$ and $2.502(13) \text{ \AA}$, respectively]. However, in the case of $\text{Cl}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$, the dithiocarbamato moieties behave as symmetrical chelating ligands, with one Sn—S bond only slightly longer than the other [average lengths $2.572(1)$ and $2.507(5) \text{ \AA}$]. The slightly longer Sn—S bond in the title compound is considerably shorter than the long Sn—S bonds [average length $2.996(3) \text{ \AA}$] reported for $\text{Me}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$, indicating the electronic influence of the Cl atoms on the Sn—S bond lengths. The dithiocarbamato S and C atoms are coplanar with Sn but the geometry of the chelation is highly distorted from the square-planar geometry (the S—Sn—S angles range from 70.9 to 160.4°) reported earlier for a number of dimethyltin(IV) dithiocarbamates.

It has been reported that the coordination geometry in dimethyltin(IV) dithiocarbamates is badly distorted from octahedral. The Me—Sn—Me angle in $\text{Me}_2\text{Sn}\{\text{S}_2\text{CN}(\text{CH}_2)_4\}_2$ (137.3°) is intermediate between *cis* and *trans* (Lockhart *et al.*, 1985) and is quite similar to that in $\text{Me}_2\text{Sn}(\text{S}_2\text{CNMe}_2)_2$ (136°) (Kimura *et al.*, 1972). Unlike the above, the Cl—Sn—Cl angle of $91.85(3)^\circ$ in $\text{Cl}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$ indicates an only slightly distorted *cis*-octahedral

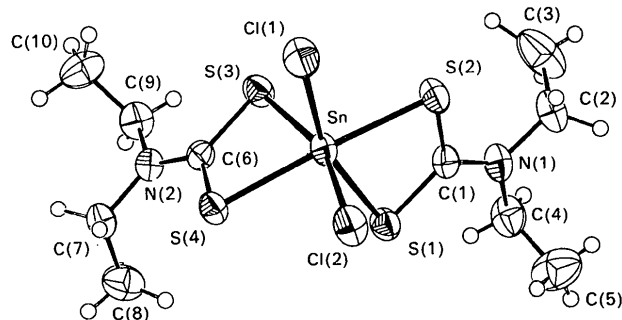


Fig. 1. A PLATON (Spek, 1990) plot of the title complex. Displacement ellipsoids are shown at the 50% probability level.