Seven-co-ordination in μ-Oxalato-bis[(di-n-propyl sulphoxide)nitratodiphenyltin(IV)]: Spectroscopic Properties and *X*-Ray Crystal Structure

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The title compound has been synthesised and its spectroscopic properties and *X*-ray structure have been studied. The structure was refined by least-squares techniques to R 4·5% for 3083 independent reflections. Crystals are triclinic, space group $P\bar{1}$, with unit-cell dimensions: a = 13·334(7), b = 11·860(6), c = 9·424(6) Å, α = 51·3(2), β = 77·5(2), γ = 71·7(2)°, Z = 1, $(C_{19}H_{24}NO_6SSn)_2$. The co-ordination around tin(IV) is pentagonal bipyramidal, the nitrate and oxalate anions and the sulphoxide molecule being equatorial, with the two phenyl rings at the apices. The oxalate ion acts as a centrosymmetric bridge between two co-ordination polyhedra. Some disorder occurs in the sulphoxide molecule, which occupies two positions around the O–Sn bond.

SEVERAL structural studies have recently been published which show that tin(IV) is able to form four-,[1-5] five-,[6-9] six-,[10-13] and, even if more rarely, seven-co-ordinate [14,15] complexes.

As a part of a study of organotin(IV) derivatives containing the nitrate group, $Ph_2Sn(NO_3)_2$ was prepared; its co-ordination products with dialkyl sulphoxides were studied in order to define the role played by the different ligands in co-ordinating to metal, particularly with respect to the possible behaviour of the NO_3 group which can be covalently or ionic bonded as well. In these compounds the nitrate group is bidentate and

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covalently bonded to metal. Addison[16] has discussed the strong oxidising power of bidentate, covalently bound nitrate groups, and this property might explain the appearance of the oxalate group, as explained later.

EXPERIMENTAL

Preparation.—Di-n-propyl sulphoxide was added at room temperature and under nitrogen, to an acetone–chloroform solution of diphenyltin(IV) dinitrate, which was prepared as described in the literature.[17,18] After several hours a few white shining prismatic crystals separated [Found: C, 44·6; H, 4·8; N, 2·8. $(C_{19}H_{24}NO_6SSn)_2$ requires C, 44·5; H, 4·7; N, 2·7%].

TABLE 1

Final atomic fractional co-ordinates and thermal parameters ‡ (Å²) with estimated standard deviations in parentheses

	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Sn	0·1975(1)	0·0376(1)	0·0372(1)	3·54(1)	3·57(1)	4·24(1)	−1·42(1)	0·07(1)	−2·04(1)
S(1)*	0·2189(2)	0·4022(2)	−0·2943(3)	6·1(1)	4·2(1)	7·0(1)	−1·1(1)	−0·7(1)	−2·6(1)
S(2)†	0·2972(4)	0·3421(6)	−0·3436(7)	4·6(2)	4·2(2)	4·4(2)	−1·9(2)	1·0(2)	−1·7(2)
O(1)	0·2808(3)	−0·1831(4)	0·3105(5)	4·8(2)	4·5(2)	5·5(2)	−1·4(1)	−0·5(1)	−2·6(1)
O(2)	0·4361(3)	−0·2190(5)	0·3895(7)	5·3(2)	7·8(3)	6·9(2)	−0·3(2)	−2·1(2)	−4·0(2)
O(3)	0·3605(3)	−0·0054(4)	0·1525(5)	4·8(2)	5·3(2)	5·6(2)	−2·0(1)	−0·2(1)	−2·9(1)
O(4)	−0·0902(3)	0·1238(4)	−0·1745(5)	3·9(1)	3·6(1)	4·6(1)	−1·7(1)	−0·4(1)	−1·5(1)
O(5)	0·0622(3)	0·1478(3)	−0·1486(4)	4·1(1)	3·6(1)	4·1(1)	−1·9(1)	−0·1(1)	−1·4(1)
O(6)	0·2460(4)	0·2433(4)	−0·1815(5)	7·8(2)	4·6(2)	5·3(2)	−3·9(2)	0·3(2)	−1·7(1)
N	0·3620(4)	−0·1377(5)	0·2873(6)	4·5(2)	5·0(2)	5·5(2)	−0·6(2)	−0·7(2)	−3·2(2)
C(1)	0·2892(4)	−0·0530(6)	−0·0976(7)	4·4(2)	4·2(2)	4·7(2)	−1·3(2)	−0·3(2)	−2·4(2)
C(2)	0·2481(5)	−0·1303(8)	−0·1293(10)	6·0(3)	6·7(3)	7·2(3)	−1·7(2)	−0·2(2)	−4·7(3)
C(3)	0·3071(6)	−0·1812(9)	−0·2308(12)	7·3(4)	8·1(4)	8·9(4)	−1·5(3)	−0·8(3)	−6·1(4)
C(4)	0·4071(6)	−0·1551(8)	−0·2985(9)	7·3(4)	6·4(3)	6·1(3)	−1·5(3)	0·3(3)	−3·7(3)
C(5)	0·4496(5)	−0·0805(8)	−0·2614(9)	5·9(3)	6·8(3)	6·5(3)	−2·1(3)	1·5(2)	−4·3(3)
C(6)	0·3919(4)	−0·0302(6)	−0·1642(8)	5·0(2)	5·1(3)	5·4(3)	−1·7(2)	0·5(2)	−2·8(2)
C(7)	0·1137(4)	0·1288(6)	0·1751(7)	5·4(2)	4·1(2)	5·1(2)	−1·7(2)	0·1(2)	−2·6(2)
C(8)	0·0306(6)	0·2533(7)	0·0930(10)	6·3(3)	5·7(3)	7·3(3)	0·0(2)	−0·5(3)	−4·1(3)
C(9)	−0·0263(7)	0·3130(9)	0·1830(12)	8·2(4)	6·3(4)	9·0(5)	0·4(3)	−0·1(3)	−4·8(4)
C(10)	−0·0029(8)	0·2479(10)	0·3592(13)	9·7(5)	7·6(4)	8·9(5)	−0·5(4)	0·3(4)	−5·8(4)
C(11)	0·0805(9)	0·1265(11)	0·4427(13)	12·5(7)	9·4(5)	7·5(4)	1·1(5)	−0·0(4)	−5·8(4)
C(12)	0·1373(7)	0·0650(10)	0·3513(11)	9·3(5)	8·4(5)	6·8(4)	0·5(4)	−0·8(3)	−4·9(4)
C(13)	−0·0090(4)	0·0771(5)	−0·0930(6)	4·1(2)	3·7(2)	3·7(2)	−1·5(1)	0·3(1)	−1·9(2)
C(14)*	0·314(1)	0·467(1)	−0·269(2)	9·4(7)	6·1(5)	14·7(9)	−3·6(5)	−0·9(7)	−4·9(6)
C(15)*	0·407(1)	0·386(2)	−0·190(2)	10·3(9)	7·8(7)	13·5(9)	−5·2(7)	−0·5(8)	−0·5(7)
C(16)*	0·481(1)	0·440(1)	−0·177(2)	9·9(7)	8·4(6)	8·0(6)	−4·7(6)	−0·9(5)	−3·5(5)
C(17)*	0·243(1)	0·472(2)	−0·536(2)	15(1)	10(1)	7(1)	−7(1)	2(1)	−4(1)
C(18)*	0·208(2)	0·396(2)	−0·584(2)	27(2)	12(1)	9(1)	−10(1)	3(1)	−6(1)
C(19)*	0·244(2)	0·415(3)	−0·742(2)	17(2)	20(2)	11(1)	−9(1)	4(1)	−11(1)
C(20)†	0·354(1)	0·445(2)	−0·331(2)	3(1)	2(1)	3(1)	−1(1)	0(1)	−1(1)
C(21)†	0·369(3)	0·388(4)	−0·121(4)	11(2)	11(2)	5(1)	−8(2)	−2(1)	−2(1)
C(22)†	0·453(3)	0·436(3)	−0·103(5)	10(2)	6(1)	10(2)	−3(1)	−2(2)	−5(1)
C(23)†	0·189(2)	0·481(3)	−0·501(3)	7(1)	4(1)	4(1)	0(1)	−1(1)	−1(1)
C(24)†	0·136(5)	0·466(6)	−0·606(7)	14(4)	13(3)	13(3)	−6(3)	2(3)	−8(3)
C(25)†	0·176(5)	0·498(6)	−0·749(7)	16(4)	11(3)	11(3)	−3(3)	−3(3)	−6(2)

* Occupancy factor 75%. † Occupancy factor 25%. ‡ Anisotropic thermal parameters are in the form: $\exp[-\frac{1}{4}(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + 2B_{23}klb^*c^*)]$.

Physical Measurements.—I.r. spectrum was measured on a Perkin-Elmer 457 spectrophotometer by the KBr technique.

X-Ray intensity data were collected on a Siemens single-crystal computer-controlled diffractometer, by the ω—2θ scan technique.

Crystal Data.—$(C_{19}H_{24}NO_6SSn)_2$, $M = 1026·4$, Triclinic, $a = 13·334(7)$, $b = 11·860(6)$, $c = 9·424(6)$ Å, $\alpha = 51·3(2)$, $\beta = 77·5(2)$, $\gamma = 71·7(2)°$, $U = 1104·7$ Å³, $D_m = 1·56$, $Z = 1$, $D_c = 1·54$, $F(000) = 518$. Cu-K_α radiation, $\lambda = 1·5418$ Å, $\mu(\text{Cu-}K_\alpha) = 106·9$ cm⁻¹. Space group $P\bar{1}$, from structural analysis.

Cell dimensions were determined from rotation and Weissenberg photographs and refined from the least-squares fit to the $(\theta,\chi,\phi)_{hkl}$ values for 16 reflections measured on the diffractometer.

Data Collection.—An elongated prismatic crystal with a mean cross-section radius of 0·064 mm, was aligned with its [001] axis along the ϕ axis of the instrument and all the reflections with $2\theta \leqslant 130°$ were collected. In this way the intensities of 3499 independent reflections were measured and 3083, having $I > 2\sigma(I)$, were considered observed and used in the analysis. The sample used for data collection decomposed appreciably in the *X*-ray beam as shown by the decreasing intensity of the standard reflection measured systematically every 20 reflections.

No correction for absorption effects was made, μ_r being (0·7) sufficiently small. The structure amplitudes were brought to an absolute scale by correlating observed with calculated values.

Structure Analysis.—The structure was solved by the heavy-atom technique, assuming the space group $P\bar{1}$ and the initial set of co-ordinates deduced for tin from the Patterson map. Two subsequent Fourier syntheses gave the co-ordinates of 28 non-hydrogen atoms, which led to R 21·3%. From the distribution of the atomic peaks, it was possible to recognise the presence of an oxalate group, which was not expected on the basis of the mode of preparation. A first refinement was carried out down to

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R 8·2% by block-diagonal least-squares with anisotropic parameters, but a subsequent ΔF map showed a remaining peak of height equivalent to an oxygen atom, but too near to sulphur (*ca.* 1·2 Å) and residuals of electron density (0·2—0·3 eÅ^{-3}) in regions close to the di-n-propyl sulphoxide molecule. From an accurate investigation of these regions and from the arrangement of the atoms, it was inferred that the di-n-propyl sulphoxide moiety was disordered, being distributed in two positions, related by rotation about the O–Sn bond and the additional peak in the ΔF map could be interpreted as a sulphur atom, with an occupancy factor of 25%; an occupancy of 75% was therefore attributed to the previously located molecule. It was also possible to locate all other atoms in the weaker component of the disordered sulphoxide molecule. A further refinement, taking this situation into account, improved R to 4·5%. No attempt was made to locate the hydrogen atoms. In applying the least-squares procedure the quantity minimized was $\Sigma w(\Delta F)^2$; unit weights were used at first, then the scheme $\frac{1}{w} = A + B|F_o| + C|F_o|^2$ was assumed, in which the coefficients A 1·960, B 0·1904, and C 0·0046 were determined by plotting ΔF *vs.* $|F_o|$. A difference-Fourier synthesis carried out at the end of the refinement showed no undesirable features.

Table 1 lists the final atomic co-ordinates and thermal parameters. The rather high σ values observed for the B_{ij} thermal parameters of the propyl carbon atoms indicate that no physical meaning can be attached to them. Observed and calculated structure-factors are given in Supplementary Publication No. SUP 20790 (15 pp., 1 microfiche).* Atomic scattering factors were taken from ref. 19.

All computations were performed on CDC 6600 computer at the Centro di Calcolo Elettronico Interuniversitario dell'Italia Nord-Orientale with programs of Immirzi.[20]

RESULTS AND DISCUSSION

I.r. Spectrum.—I.r. spectroscopic data for the 4000—250 cm^{-1} region are given in Table 2. The vibrational frequencies of interest are those due to the phenyl rings, nitrate and oxalate anions, and the di-n-propyl sulphoxide group: in particular the nitrate absorption bands indicate that this group is bidentate and covalently bonded [16] to the metal, and the oxalate group exhibits symmetric and antisymmetric carboxy-stretching frequencies consistent with chelate behaviour.[21]

TABLE 2

Selected i.r. absorption frequencies (cm^{-1}) with their tentative assignments

3075w	ν(CH)	1460m	β(CH)
3050w	ν(CH)	1430s	ν(C⁚C)
2965m	ν(CH)	1382vs	ν_s(COO)
2930sh	ν(CH)	1310m	β(CH)
2870w	ν(CH)	1275m	ν(NO) ν(C·O) + ∂(O·C⁚O)
1620br, vs	ν_{as}(NO$_2$) ν_{as}(COO)	998sh	π(NO$_3$)
1580sh	ν(C⁚C)	960s	ν(S⁚O)
1568m	ν(C⁚C)	798s	∂(O·C⁚O)
1495m	ν(NO)	725s	β(CH)
1480m	ν(C⁚C)	690s	β(CH)

w = Weak, m = medium, sh = shoulder, br = broad, s = strong, vs = very strong.

The ν(SO) band of di n-propyl sulphoxide is shifted toward lower-frequency values with respect to the free ligand,[22] in agreement with co-ordination through oxygen atom.

In the 600—250 cm^{-1} region there are several weak bands which are difficult to assign with certainty.

X-*Ray Structure.*—As can be seen from Figure 1, which represents a clinographic projection of the structure, the main features from the X-ray analysis are the seven-co-ordination around metal and the presence of an oxalate anion bridging two metal atoms. As was observed in the introduction, this oxalate ion must be derived from an oxidation process probably involving ethanol, present in the chloroform solvent, and due to the strong oxidising power of the covalently bound bidentate NO$_3^-$.

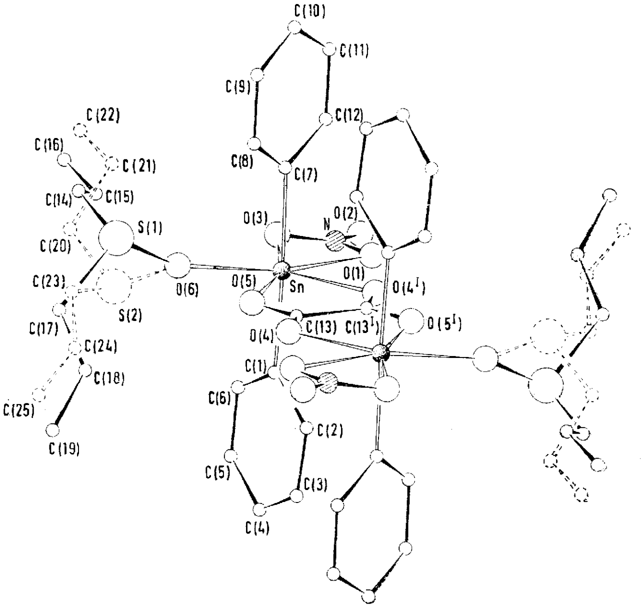

FIGURE 1 Clinographic projection of the structure. The di-n-propyl sulphoxide molecule is disordered: full line indicates 75%, dotted line 25% occupancy

Tin(IV) is surrounded by two oxygen atoms from a nitrate ion, an oxygen atom from a sulphoxide molecule, two oxygen atoms from an oxalate ion, and two carbon atoms from two phenyl rings in a pentagonal bipyramidal arrangement. The five oxygen atoms involved in co-ordination lie at the vertices of a pentagon centred on the tin atom (Figure 2), with O–Sn–O angles in the range 53·0—81·6°. The pentagonal girdle is planar (Table 3), the largest deviation from the mean plane being 0·04 Å for O(1) and O(2). The metal atom is practically coplanar (0·04 Å) with the five equatorial

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* See Notice to Authors No. 7 in *J.C.S. Dalton*, 1972, Index issue.

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atoms. The pentagonal bipyramid co-ordination polyhedron of tin is completed by two phenyl carbon atoms, C(1) and C(7), which occupy the axial positions forming C–Sn bonds which are nearly perpendicular (87·1 and 90·0°) to the equatorial plane. This type of bonding geometry for tin(IV) is rather unusual, but has been recently observed for two other tin(IV) complexes: chlorotris(tropolonato)tin and hydroxotris(tropolonato)-tin.[14]

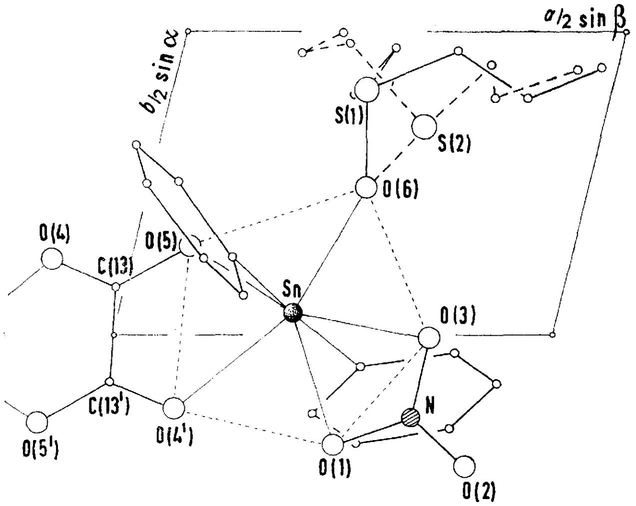

FIGURE 2 Diagramatic projection of an asymmetric unit along [001]

TABLE 3

Main least-squares planes in the structure

Plane (1): O(1), O(3), O(4$^{\mathrm{I}}$), O(5), O(6)
$0{\cdot}4904X - 0{\cdot}7332Y - 0{\cdot}4711Z = 0{\cdot}0432$
Plane (2): N(1), O(1)—(3)
$0{\cdot}4144X - 0{\cdot}7080Y - 0{\cdot}5719Z = 0{\cdot}3977$
Plane (3): C(1)—(6)
$-0{\cdot}4122X + 0{\cdot}3394Y - 0{\cdot}8455Z = -0{\cdot}9006$
Plane (4): C(7)—(12)
$0{\cdot}6245X + 0{\cdot}6885Y - 0{\cdot}3687Z = 0{\cdot}25361$

X, *Y*, *Z*, are the co-ordinates in Å referred to orthogonal axes, and referred to the *x*, *y*, *z*, triclinic ones by applying the matrix: $\sin\gamma\ 0\ -\sin\alpha\cos\beta^{*}\ |\ \cos\gamma\ 1\ \cos\alpha\ |\ 0\ 0\ \sin\alpha\sin\beta^{*}$. Roman numeral as superscript refer to the *x*,*y*,*z*, equivalent position.

Table 4 lists bond distances and angles. The Sn–O bonds are not all equal: the shortest involving the sulphoxide molecule, is a normal single bond, and lies at the upper limit of the range usually found (2·05—2·17 Å) for Sn–O distances in seven-co-ordinate tin(IV) complexes;[14,15] the others are probably lengthened by some effect such as interligand repulsions.

The oxalate ion connects two adjacent co-ordination polyhedra through two O–C–O bridges, giving rise to dimers. The two tin atoms bridged by the oxalate ion lie practically in the oxalate plane, the dihedral angle formed by the chelation ring and the oxalate group being 177·3°. As is frequently observed with oxalate structures, the asymmetric unit consists of one-half oxalate ion, since its centre of gravity is a centre of symmetry in the space group. The two C–O distances differ significantly in length, the longer one taking part in a short O–Sn bond.

TABLE 4

Bond distances (Å) and angles (deg.) with standard deviations in parentheses

(*a*) In the co-ordination polyhedron			
Sn–O(1)	2·388(6)	Sn–O(6)	2·178(6)
Sn–O(3)	2·408(6)	Sn–C(1)	2·115(7)
Sn–O(4$^{\mathrm{I}}$)	2·282(5)	Sn–C(7)	2·116(8)
Sn–O(5)	2·248(5)		
O(1)–Sn–O(3)	53·0(2)	O(5)–Sn–C(1)	91·3(2)
O(1)–Sn–O(4$^{\mathrm{I}}$)	73·2(1)	O(6)–Sn–C(1)	87·1(2)
O(3)–Sn–O(6)	79·2(2)	O(1)–Sn–C(7)	91·4(2)
O(4$^{\mathrm{I}}$)–Sn–O(5)	73·0(1)	O(3)–Sn–C(7)	89·8(2)
O(5)–Sn–O(6)	81·6(2)	O(4$^{\mathrm{I}}$)–Sn–C(7)	90·0(2)
O(1)–Sn–C(1)	87·2(2)	O(5)–Sn–C(7)	91·5(2)
O(3)–Sn–C(1)	87·1(2)	O(6)–Sn–C(7)	91·6(2)
O(4$^{\mathrm{I}}$)–Sn–C(1)	92·4(2)	C(1)–Sn–C(7)	176·8(2)
(*b*) In the nitrate ion			
N–O(1)	1·275(8)	N–O(3)	1·255(8)
N–O(2)	1·219(7)		
O(1)–N–O(2)	121·6(6)	N–O(1)–Sn	95·7(3)
O(1)–N–O(3)	115·6(4)	N–O(3)–Sn	95·3(3)
O(2)–N–O(3)	122·8(6)		
(*c*) In the oxalate ion			
O(4)–C(13)	1·233(6)	C(13)–C(13$^{\mathrm{I}}$)	1·540(8)
O(5)–C(13)	1·271(7)		
O(4)–C(13)–O(5)	125·1(5)	C(13)–O(5)–Sn	116·8(3)
O(4)–C(13)–C(13$^{\mathrm{I}}$)	119·0(5)	C(13$^{\mathrm{I}}$)–O(4$^{\mathrm{I}}$)–Sn	115·2(4)
O(5)–C(13)–C(13$^{\mathrm{I}}$)	115·9(4)		
(*d*) In the di-n-propyl sulphoxide			
O(6)–S(1)	1·430(7)	O(6)–S(2)	1·409(8)
S(1)–C(14)	1·80(2)	S(2)–C(20)	1·69(3)
S(1)–C(17)	1·86(1)	S(2)–C(23)	1·84(3)
C(14)–C(15)	1·33(2)	C(20)–C(21)	1·68(4)
C(15)–C(16)	1·39(3)	C(21)–C(22)	1·49(6)
C(17)–C(18)	1·45(3)	C(23)–C(24)	1·45(8)
C(18)–C(19)	1·35(3)	C(24)–C(25)	1·19(8)
O(6)–S(1)–C(14)	109·6(6)	O(6)–S(2)–C(20)	114·7(7)
O(6)–S(1)–C(17)	108·2(7)	O(6)–S(2)–C(23)	104·0(9)
C(14)–S(1)–C(17)	101·8(8)	C(20)–S(2)–C(23)	103(1)
S(1)–C(14)–C(15)	126(2)	S(2)–C(20)–C(21)	116(2)
C(14)–C(15)–C(16)	125(2)	C(20)–C(21)–C(22)	116(3)
S(1)–C(17)–C(18)	116(1)	S(2)–C(23)–C(24)	126(4)
C(17)–C(18)–C(19)	119(2)	C(23)–C(24)–C(25)	118(6)
S(1)–O(6)–Sn	147·4(3)	S(2)–O(6)–Sn	158·3(5)
(*e*) In the phenyl rings			
C(1)–C(2)	1·40(1)	C(7)–C(8)	1·39(1)
C(2)–C(3)	1·41(1)	C(8)–C(9)	1·39(1)
C(3)–C(4)	1·39(1)	C(9)–C(10)	1·39(1)
C(4)–C(5)	1·42(1)	C(10)–C(11)	1·37(2)
C(5)–C(6)	1·37(1)	C(11)–C(10)	1·42(2)
C(6)–C(1)	1·41(1)	C(12)–C(7)	1·39(1)
C(1)–C(2)–C(3)	120·7(7)	C(7)–C(8)–C(9)	121·1(7)
C(2)–C(3)–C(4)	119·6(10)	C(8)–C(9)–C(10)	120·9(9)
C(3)–C(4)–C(5)	119·5(9)	C(9)–C(10)–C(11)	119·4(11)
C(4)–C(5)–C(6)	120·8(7)	C(10)–C(11)–C(12)	119·5(9)
C(5)–C(6)–C(1)	120·4(8)	C(11)–C(12)–C(7)	121·5(9)
C(6)–C(1)–C(2)	119·0(6)	C(12)–C(7)–C(8)	117·6(8)
C(6)–C(1)–Sn	119·9(6)	C(12)–C(7)–Sn	121·9(6)
C(2)–C(1)–Sn	121·1(4)	C(8)–C(7)–Sn	120·5(5)

The nitrate group is bidentate through two oxygen atoms, as suggested also by the i.r. spectrum, and is perfectly planar (Table 3). The two N–O distances involving donor oxygen atoms (1·255 and 1·275 Å) are slightly shorter than those quoted[23] for asymmetric

[23] C. D. Garner, J. Hilton, and S. C. Wallwork, *Acta Cryst.*, 1969, **A25**, *S*104.

bidentate co-ordination (1·29 and 1·31 Å), but also slightly longer than the third N–O (1·219 Å) bond; as a consequence of this last fact the O–N–O angle opposite this bond is narrower than the other two. The values of the Sn–O–N angles (95·3 and 95·7°) are in agreement with the nitrate ion being bidentate, since that angle tends to 110°, and is decreased when the ligand is bidentate and increased when it is unidentate.[23]

Both benzene rings, which are *trans* with respect to the equatorial plane, are planar as expected (Table 3): the metal atom is out of the C(1)—(6) plane by 0·14 Å, but it is nearly coplanar with the C(7)—(12) plane, the displacement being only 0·04 Å. The orientation of the two aromatic rings can be defined by the dihedral angles they form with the equatorial plane (93·0 and 91·4°) and by the angle of rotation between them (73·2°).

The di-n-propyl sulphoxide molecule co-ordinates through the oxygen atom and the $\mathrm{Pr^n{}_2S}$ part is disordered into two positions around the Sn–O bond, the oxygen atom is not disordered, since it is strongly bonded to metal. The configuration of the two *sulph*oxide groups is pyramidal, the perpendicular distances from the apical sulphur atoms to the OCC base planes are 0·63 for S(1) and 0·59 Å for S(2). The departures from expected values for bond distances and angles of the carbon atoms of the propyl chains are large, but not significant owing to their disordered nature.

Packing is consistent with van der Waals interactions.

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