represented to follow the order $G < R_2 < R_1$, where R_1 and R_2 are the glycinato rings coordinated to Co through O(4) and O(6) respectively. This strain makes the Co—O(4) bond length [1·947 (3) Å] longer than Co—O(6) [1·857 (3) Å]. The possible hydrogen bonds are given in Table 3.

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Structure of Triphenyltin(IV) 2-Thiophenecarboxylate

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Abstract. $[(C_6H_5)_3SnOC(O)C_4H_3S]$, $M_r = 477{\cdot}15$, monoclinic, $P2_1/n$, $a = 14{\cdot}237\ (3)$, $b = 11{\cdot}785\ (2)$, $c = 13{\cdot}448\ (2)$ Å, $\beta = 116{\cdot}65\ (1)°$, $V = 2017\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}571$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 13{\cdot}8$ cm^{-1}, $F(000) = 952$, $T = 295\ (1)$ K, $R = 0{\cdot}041$ for 2617 $[I > 3\sigma(I)]$ reflections. The Sn is four-coordinate and the tetrahedral geometry is distorted owing to an intramolecular tin–carbonyl oxygen contact of 2·768 (4) Å.

Introduction. Triorganotin(IV) alkanoates are generally polymeric because of carboxylate bridging which results in the *trans*-C_3SnO_2 trigonal bipyramidal geometry at tin (Davies & Smith, 1982), especially in the absence of other donor atoms in the carboxylate unit (Ng, Chen Wei & Kumar Das, 1988). The triphenyltin arylcarboxylates are a fairly consistent series of four-coordinate tin structures (Harrison, Lambert, King & Majee, 1983; Holmes, Day, Chandrasekhar, Vollano & Holmes, 1986*a*; Swisher, Vollano, Chandrasekhar, Day & Holmes, 1984; Vollano, Day, Rau, Chandrasekhar & Holmes, 1984) whose distortion from idealized geometry arises from the short intramolecular acyl oxygen–tin (2·463–2·861 Å) distances which, although less than the sum of the van der Waals radii (3·70 Å) of tin and oxygen, are nevertheless longer than the covalent Sn—O bonds (2·048–2·115 Å). On the basis of infrared and tin-119*m* Mössbauer data, the heterocyclic analogues, triphenyltin 2-thiophene- and 2-furan- (Sandhu & Verma, 1986) carboxylates are reported to be four-coordinate; the report prompted the present crystal study of triphenyltin 2-thiophenecarboxylate.

Experimental. Crystals of triphenyltin 2-thiophenecarboxylate were grown from an alcoholic solution of triphenyltin hydroxide and 2-thiophenecarboxylic acid. A crystal measuring 0·32 × 0·15 × 0·16 mm was mounted on an Enraf–Nonius CAD-4 diffractometer for the X-ray data collection. 25 reflections ($15° < 2\theta < 18°$) were used to determine the cell constants. Lorentz–polarization, linear decay based on repeatedly measuring three independent reflections (from 0·987 to 1·000 on I), reflection averaging (agreement on I 1·8%) and empirical absorption (from 7·21% to 0·08% on I) corrections were applied. The maximum 2θ was 50·0° with the hkl ranges being h −16 to 15, k 0 to 13 and l 0 to 15. Of the 3887 total reflections, 3721 were unique

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and 2617 with $|F_o|^2 > 3\sigma(|F_o|^2)$ were used in the least-squares refinements. The structure was solved by the Patterson method; H atoms were not included; the number of parameters refined was 244. The final unweighted agreement factor was 0·041 and the weighted agreement factor 0·055; the 'fudge factor' was 0·04 and the goodness of fit was 1·70. The ratio of the maximum least-squares shift to e.s.d. in the final refinement cycle was less than 0·01. The minimization function was set at $\sum w(|F_o| - |F_c|)^2$. The final difference Fourier map was almost featureless, with the highest peak at 0·62 (9) and the lowest peak at −0·44 (9) e Å^{-3}; $w = 1/\sigma|F_o|^2$. All calculations were carried out on a VAX II microcomputer using the Enraf–Nonius *SDP* (Frenz, 1985) software. The atomic coordinates are listed in Table 1 and the bond distances and angles in Table 2.*

Table 1. *Atomic coordinates for triphenyltin 2-thiophenecarboxylate*

	x	y	z	B_{eq}(Å^2)
Sn	0·95725 (3)	0·23607 (3)	0·19762 (3)	3·547 (8)
S	1·2929 (1)	0·4940 (2)	0·4751 (2)	5·73 (5)
O(1)	1·0119 (3)	0·3628 (4)	0·3175 (3)	4·6 (1)
O(2)	1·1589 (3)	0·3229 (4)	0·3062 (4)	5·0 (1)
C(1)	1·1117 (4)	0·3784 (5)	0·3467 (5)	4·1 (1)
C(11)	1·0396 (4)	0·0830 (5)	0·2666 (5)	3·7 (1)
C(12)	1·0664 (5)	0·0538 (6)	0·3753 (5)	5·2 (2)
C(13)	1·1205 (5)	−0·0500 (7)	0·4188 (6)	6·1 (2)
C(14)	1·1475 (5)	−0·1205 (6)	0·3521 (6)	6·2 (2)
C(15)	1·1198 (5)	−0·0903 (6)	0·2413 (6)	6·1 (2)
C(16)	1·0666 (5)	0·0121 (6)	0·2001 (6)	4·9 (2)
C(21)	0·9585 (4)	0·3004 (5)	0·0518 (5)	3·6 (1)
C(22)	0·8632 (5)	0·3288 (6)	−0·0378 (5)	4·6 (2)
C(23)	0·8636 (5)	0·3754 (6)	−0·1333 (6)	5·7 (2)
C(24)	0·9563 (6)	0·3900 (6)	−0·1423 (6)	5·6 (2)
C(25)	1·0518 (5)	0·3619 (6)	−0·0523 (5)	5·6 (2)
C(26)	1·0524 (4)	0·3162 (6)	0·0449 (5)	4·8 (2)
C(31)	0·8054 (4)	0·2317 (5)	0·1912 (4)	3·5 (1)
C(32)	0·7701 (4)	0·1341 (5)	0·2224 (5)	4·4 (2)
C(33)	0·6701 (5)	0·1322 (6)	0·2208 (6)	5·2 (2)
C(34)	0·6072 (5)	0·2280 (6)	0·1873 (5)	5·0 (2)
C(35)	0·6409 (5)	0·3261 (6)	0·1557 (5)	5·0 (2)
C(36)	0·7394 (4)	0·3284 (6)	0·1557 (5)	4·4 (2)
C(41)	1·1615 (4)	0·4705 (5)	0·4287 (5)	4·1 (1)
C(42)	1·1148 (4)	0·5463 (5)	0·4749 (4)	3·6 (1)
C(43)	1·1944 (5)	0·6221 (6)	0·5486 (5)	5·6 (2)
C(44)	1·2914 (5)	0·6027 (7)	0·5562 (5)	5·8 (2)

$B_{eq} = (4/3)[a^2B_{1,1} + b^2B_{2,2} + c^2B_{3,3} + ab(\cos\gamma)B_{1,2} + ac(\cos\beta)B_{1,3} + bc(\cos\alpha)B_{2,3}]$.

Discussion. The molecular structure of triphenyltin 2-thiophenecarboxylate is depicted in Fig. 1. The monomeric units are well separated in the unit cell. The three *ipso*-carbons of the phenyl and the O of the

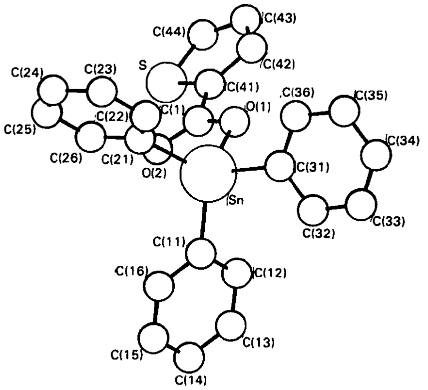

Fig. 1. A molecule of triphenyltin 2-thiophenecarboxylate.

Table 2. *Bond distances* (Å) *and bond angles* (°) *for triphenyltin 2-thiophenecarboxylate*

Sn—O(1)	2·076 (4)	Sn—C(11)	2·125 (6)	Sn—C(21)	2·110 (7)
Sn—C(31)	2·125 (6)	C(11)—C(12)	1·379 (9)	C(12)—C(13)	1·42 (1)
C(13)—C(14)	1·39 (1)	C(14)—C(15)	1·41 (1)	C(15)—C(16)	1·401 (9)
C(16)—C(11)	1·40 (1)	C(21)—C(22)	1·393 (7)	C(22)—C(23)	1·40 (1)
C(23)—C(24)	1·39 (1)	C(24)—C(25)	1·395 (8)	C(25)—C(26)	1·41 (1)
C(26)—C(21)	1·39 (1)	C(31)—C(32)	1·393 (9)	C(32)—C(33)	1·41 (1)
C(33)—C(34)	1·39 (1)	C(34)—C(35)	1·39 (1)	C(35)—C(36)	1·40 (1)
C(36)—C(31)	1·416 (8)	O(1)—C(1)	1·307 (7)	C(1)—O(2)	1·226 (9)
C(1)—C(41)	1·482 (8)	C(41)—C(42)	1·413 (9)	C(42)—C(43)	1·433 (8)
C(43)—C(44)	1·36 (1)	C(44)—S	1·688 (6)	S—C(41)	1·708 (6)

O(1)—Sn—C(11)	109·3 (2)	O(1)—Sn—C(21)	107·9 (2)	O(1)—Sn—C(31)	93·9 (3)
C(11)—Sn—C(21)	118·5 (3)	C(11)—Sn—C(31)	110·5 (2)	C(21)—Sn—C(31)	113·8 (2)
Sn—O(1)—C(1)	108·2 (4)	Sn—C(11)—C(12)	120·7 (5)	Sn—C(11)—C(16)	119·0 (4)
C(11)—C(12)—C(13)	119·4 (7)	C(12)—C(13)—C(14)	121·1 (7)	C(13)—C(14)—C(15)	120·3 (7)
C(14)—C(15)—C(16)	118·8 (8)	C(15)—C(16)—C(11)	121·1 (7)	C(16)—C(11)—C(12)	120·3 (6)
Sn—C(21)—C(22)	118·7 (5)	Sn—C(21)—C(26)	121·2 (4)	C(21)—C(22)—C(23)	119·0 (7)
C(22)—C(23)—C(24)	121·6 (6)	C(23)—C(24)—C(25)	119·3 (7)	C(24)—C(25)—C(26)	119·5 (7)
C(25)—C(26)—C(21)	120·4 (5)	C(26)—C(21)—C(22)	120·1 (6)	Sn—C(31)—C(32)	120·4 (4)
Sn—C(31)—C(36)	120·2 (5)	C(31)—C(32)—C(33)	120·4 (6)	C(32)—C(33)—C(34)	119·4 (7)
C(33)—C(34)—C(35)	121·1 (7)	C(34)—C(35)—C(36)	119·9 (6)	C(35)—C(36)—C(31)	119·8 (6)
C(36)—C(31)—C(32)	119·4 (6)	O(1)—C(1)—O(2)	122·0 (5)	O(1)—C(1)—C(41)	114·8 (6)
O(2)—C(1)—C(41)	123·2 (6)	C(1)—C(41)—S	118·1 (5)	C(1)—C(41)—C(42)	128·9 (5)
C(41)—C(42)—C(43)	108·4 (6)	C(42)—C(43)—C(44)	114·2 (7)	C(43)—C(44)—S	112·7 (5)
C(44)—S—C(41)	91·8 (3)	S—C(41)—C(42)	113·0 (4)		

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51524 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

carboxylate groups make up the corners of the tetrahedron around the Sn and there is a weak carbonyl O···Sn contact [2·768 (4) Å]. The C—Sn—C angles are opened up [110·5 (2), 113·8 (2), 118·5 (3)°] whereas the O—Sn—C angles are compressed [93·9 (3), 107·9 (2), 109·3 (2)°]. The thienyl ring is flat [sum of internal angles is 540 (3)°] and is coplanar with the C(=O)—O [dihedral angle = 4 (3)°] fragment. The aromatic ring and carboxylate group in the corresponding triphenyltin benzoate esters are also coplanar with the exception of polymeric triphenyltin 2-chlorobenzoate, whose two planes are twisted by about 60° (Holmes, Day, Chandrasekhar, Vollano & Holmes, 1986*b*).

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Structure of Triphenyltin(IV) 3-Pyridinecarboxylate

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Abstract. $[(C_6H_5)_3SnOC(O)C_5H_4N]$, $M_r = 472·11$, tetragonal, $P4_1$, $a = 12·075$ (2), $c = 14·629$ (2) Å, $V = 2133$ (1) Å^3, $Z = 4$, $D_x = 1·469$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 12·2$ cm^{-1}, $F(000) = 944$, $T = 296$(1)K, final $R = 0·028$ for 1427 reflections. The geometry at Sn is *trans*-C_3SnNO trigonal bipyramidal and the Sn is displaced out of the equatorial plane by 0·118 (1) Å in the direction of the O. The molecules are linked by intermolecular Sn←:N [2·568 (7) Å] bridges. The pyridine ring of one molecule and the pyridine ring of the adjacent molecule are coplanar [dihedral angle 179 (6)°].

Introduction. Triorganotin esters of carboxylic acids are often five-coordinate polymers because of carboxylate bridging but the benzoate-type triphenyltin esters are generally monomeric (Ng, Kumar Das, van Meurs, Schagen & Straver, 1989). Stannyl esters of 2-pyrrole- (Sandhu & Verma, 1986) and 2-pyridine- (Harrison & Phillips, 1975) carboxylic acids appear to be carboxylate-bridged on spectroscopic evidence (IR, tin-119*m* Mössbauer) but nitrogen-bridged structures have been inferred for tri-*n*-butyltin 3- and 4-pyridinecarboxylates (Allen, Brooks, Formstone, Crowe & Smith, 1978). In the crystal structure of trimethyltin 2-pyridinecarboxylate monohydrate, the water is coordinated to tin and the molecules are hydrogen bonded into a three-dimensional lattice (Harrison & Phillips, 1979). A stretched helical nitrogen-bridged polymeric configuration is predicted for the title compound, triphenyltin 3-pyridinecarboxylate (nicotinate), from its variable-temperature Mössbauer spectrum ($80 \leq T \leq 130$ K; $a\ -2·02 \times 10^{-1}$ K^{-1}) (Ng & Kumar Das, 1988). The present crystal-structure study was aimed at corroborating the spectral finding.

Experimental. The title compound was prepared by mixing stoichiometric quantities of nicotinic acid and

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