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(*N*-Maleoylglycinato)trimethyltin(IV)

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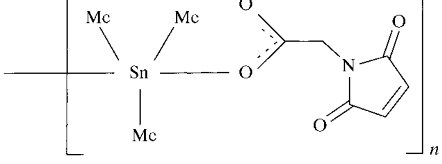
The Sn atom in the crystal structure of the title compound, *catena*-poly[trimethyltin-μ-[(2,5-dioxo-2,5-dihydropyrrol-1-yl)acetato-*O*:*O*′]], [Sn(CH$_3$)$_3$(C$_6$H$_4$NO$_4$)], adopts a distorted trigonal bipyramidal coordination geometry with three methyl groups defining the trigonal plane [mean Sn—C 2.117 (11) Å] and the axial positions occupied by O atoms from different carboxylate groups, with significantly different Sn—O bond lengths [2.207 (5) and 2.358 (6) Å]. The structure forms a polymeric chain of complex molecules linked *via* carboxylate moieties.

Comment

In the past two decades, organotin carboxylates have received much attention because of their extensive applications in different fields of life science (Davis & Smith, 1982; Tagliavini, 1992; Brimah *et al.*, 1994), especially biocidal applications, utilizing the antitumour and anticancer activities of such compounds (Gielen *et al.*, 1994; de Vos *et al.*, 1998). Accordingly, and in view of our continuous interest in the synthesis, characterization, biological applications and crystal structures of organotin carboxylates (Danish *et al.*, 1995; Parvez *et al.*, 1997; Parvez, Ali, Mazhar, Bhatti & Khokhar, 1999; Parvez, Ali, Mazhar, Bhatti & Choudhary, 1999), we have prepared a new organotin derivative of 2-maleimidoacetic acid, commonly known as *N*-maleoylglycine. In this paper, we now report the crystal structure of (*N*-maleoylglycinato)trimethyltin(IV), (I).



(I)

The structure of (I) is presented in Fig. 1. The Sn atom is bonded to three methyl groups in equatorial positions with Sn—C distances [mean 2.117 (11) Å] that are essentially equal within experimental uncertainty and that are in agreement with the values reported for related structures (Allen *et al.*, 1983). The axial positions are occupied by O atoms from the carboxylate residues, with a nearly linear O—Sn—O angle of 172.90 (19)°. The intramolecular distance Sn1—O1 [2.207 (5) Å] is significantly shorter than the intermolecular distance Sn1—O2^{i} [2.358 (6) Å; symmetry code: (i) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$], indicating that the former is a covalent bond and the latter a coordinate bond. The Sn atom has distorted trigonal bipyramidal coordination geometry, with the Sn atom 0.084 (6) Å out of the equatorial plane formed by the three methyl C atoms towards the more strongly bound O1 atom. This trend is in line with similar structures reported by our laboratories, as mentioned above.

The molecular dimensions in the ligand, *N*-maleoylglycine, are normal, with the five-membered ring essentially planar [maximum deviation: N1 0.035 (5) Å] and with slightly pyramidal geometry about N1. The structure is composed of infinite chains of (I) running along the *b* axis.

A few examples of crystal structures containing triorganotin complexes of protected compounds forming polymeric chains similar to (I) are: (3-indolylacetato-*O*,*O*′)tri-*n*-butyltin (Molloy *et al.*, 1987), (glutamato-*O*,*O*′)trimethyltin (Huber *et al.*, 1989), [3-(2-thienyl)-2-propenoato]triethyltin (Danish *et al.*, 1995), 2-[(2,3-dimethylphenyl)aminobenzoato-*O*,*O*′]trimethyltin (Tahir *et al.*, 1997), (picolinato *N*-oxide)triphenyltin and (nicotinato *N*-oxide)triphenyltin (Ng & Kumar Das, 1995), triphenyl(3-ureidopropionato-*O*,*O*′)tin (Lo *et al.*, 1991) and (*N*-salicylidene-6-aminohexanoato-*O*,*O*′)triphenyltin (Toong *et al.*, 1992).

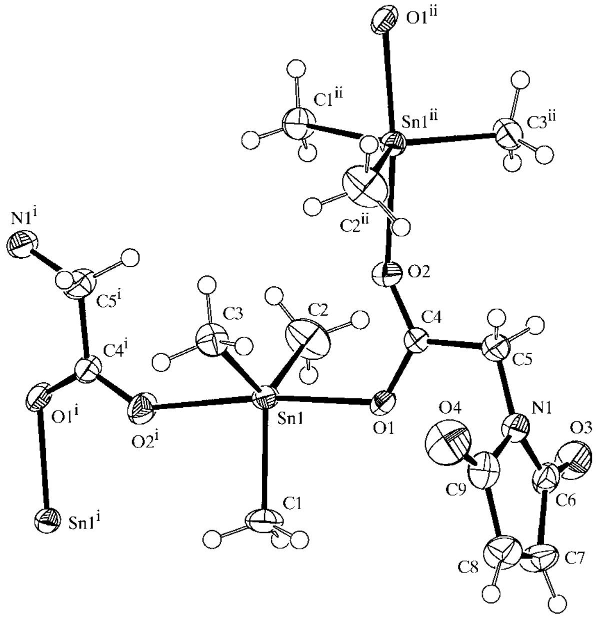


Figure 1
*ORTEP*II (Johnson, 1976) drawing of (I) with the atomic numbering scheme. Displacement ellipsoids have been plotted at the 40% probability level and H atoms assigned arbitrary radii. [Symmetry codes: (i) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$; (ii) $1 - x, -\frac{1}{2} + y, \frac{3}{2} - z$.]

Experimental

N-Maleoylglycine was prepared according to the literature method of Rich *et al.* (1975). Solid maleamic acid (8.4 mmol) was suspended in dry toluene and treated with triethylamine (17.0 mmol). The mixture was refluxed with vigorous stirring for 4 h. The water formed was continuously removed *via* Dean–Stark apparatus. After cooling, toluene was removed from the orange layer, trimethyltin chloride (8.4 mmol) was added in toluene and the mixture was refluxed for 3–4 h. On cooling, triethylammonium chloride was filtered off, toluene removed using a rotary evaporator, and the mass left was crystallized from dichloromethane/*n*-hexane (1:1) solution to yield the title compound.

Crystal data

$[Sn(CH_3)_3(C_6H_4NO_4)]$
$M_r = 317.89$
Monoclinic, $P2_1/c$
$a = 6.5848$ (15) Å
$b = 9.991$ (4) Å
$c = 19.688$ (6) Å
$\beta = 93.31$ (3)°
$V = 1293.1$ (7) Å^3
$Z = 4$
$D_x = 1.633$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta = 10.0$–15.0°
$\mu = 1.971$ mm^{-1}
$T = 170$ (2) K
Block, colourless
0.58 × 0.30 × 0.28 mm

Data collection

Rigaku AFC-6*S* diffractometer
ω–2θ scans
Absorption correction: empirical using intensity measurements (ψ scans, 3 reflections; North *et al.*, 1968)
$T_{\min} = 0.373$, $T_{\max} = 0.576$
3235 measured reflections
2985 independent reflections
2205 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.054$
$\theta_{\max} = 27.54$°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 12$
$l = -25 \rightarrow 25$
3 standard reflections every 200 reflections intensity decay: <0.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.147$
$S = 1.202$
2985 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 11.0866P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.0001$
$\Delta\rho_{\max} = 1.27$ e Å^{-3}
$\Delta\rho_{\min} = -1.38$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0006 (5)

Most H atoms were visible in difference maps, but were placed in idealized positions (0.95–0.99 Å) for refinement, which utilized a riding model. A torsional parameter was refined for each methyl group. The final difference map was essentially free of any chemically significant features, with the highest electron density 0.9 Å from the Sn atom. There are 51 Å^3 voids in the structure at the inversion centres; the final difference map showed no significant electron density in those regions.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1994). Program(s) used to solve structure: *SAPI*91 (Fan, 1991). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*97.

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Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.116 (8)	O2—C4	1.248 (9)
Sn1—C2	2.131 (9)	O3—C6	1.202 (10)
Sn1—C3	2.104 (8)	O4—C9	1.203 (11)
Sn1—O1	2.207 (5)	N1—C6	1.378 (11)
Sn1—O2^{i}	2.358 (6)	N1—C9	1.393 (11)
O1—C4	1.260 (9)	N1—C5	1.446 (10)
C1—Sn1—C2	117.7 (4)	C3—Sn1—O2^{i}	89.8 (3)
C1—Sn1—C3	118.0 (4)	O1—Sn1—O2^{i}	172.90 (19)
C2—Sn1—C3	123.9 (4)	C4—O1—Sn1	119.5 (5)
C1—Sn1—O1	88.0 (3)	C4—O2—Sn1^{ii}	143.1 (5)
C2—Sn1—O1	93.4 (4)	C6—N1—C9	109.6 (7)
C3—Sn1—O1	95.0 (3)	C6—N1—C5	123.7 (7)
C1—Sn1—O2^{i}	85.1 (3)	C9—N1—C5	123.5 (8)
C2—Sn1—O2^{i}	88.2 (4)		

Symmetry codes: (i) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$; (ii) $1 - x, -\frac{1}{2} + y, \frac{3}{2} - z$.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1244). Services for accessing these data are described at the back of the journal.

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