Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Di-*n*-butylbis(thiophene-2-carboxylato-*O*,*O*′)tin(IV)

Abderrahmane Yahyi,[a] Abdelkader Et-touhami,[a] Ismail Zidane,[a] Nour-eddine Benchat,[a] Brahim El-Bali[b] and Michael Bolte[c]*

[a]Laboratoire de Chimie Organique Physique, Faculté des Sciences, Oujda, Morocco, [b]Laboratoire des Materiaux et Protection de l'Environnement, Département de Chimie, Faculté des Sciences DM, BP1796, Fès, Morocco, and [c]Institut für Organische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Straße 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail:
bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.024
wR factor = 0.061
Data-to-parameter ratio = 24.0

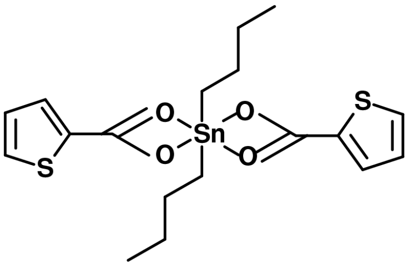
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[\mathrm{Sn(C_4H_9)_2(C_5H_3O_2S)_2}]$, crystallizes with two molecules in the asymmetric unit, differing just in the orientation of one of the n-butyl groups. The carboxylate groups asymmetrically chelate the Sn atom.

Received 15 January 2001
Accepted 16 January 2001
Online 19 January 2001

Comment

Organotin carboxylates have been the subject of several investigations in recent years (Meriem *et al.*, 1990; Meunier-Piret *et al.*, 1993; Gielen *et al.*, 1995). They are of interest because of their potential pharmaceutical applications, especially their significant antitumoral activity (Meriem *et al.*, 1991). We have performed the crystal structure determination of the title compound, (I), in order to determine its conformation. It crystallizes with two molecules in the asymmetric unit, which differ only in the orientation of one n-butyl group. The thiophenecarboxylate groups binding the same Sn atom are nearly coplanar and are asymmetrically chelating.



(I)

Experimental

The title compound was prepared by refluxing a suspension of 10 mmol dibutyltin oxide in a solution of 20 mmol 2-thiophenic acid in a mixture of 150 ml chloroform and 50 ml ethanol for 5 h. The product was distilled off and evaporated under vacuum. Crystals suitable for structure determination were obtained from an ethanol solution.

Crystal data

$[\mathrm{Sn(C_4H_9)_2(C_5H_3O_2S)_2}]$
M_r = 487.18
Monoclinic, $P2_1/c$
a = 18.238 (2) Å
b = 21.984 (3) Å
c = 10.586 (1) Å
β = 94.051 (6)°
V = 4233.8 (8) Å^3
Z = 8

D_x = 1.529 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 507 reflections
θ = 2–25°
μ = 1.42 mm^{-1}
T = 173 (2) K
Plate, colourless
0.50 × 0.40 × 0.20 mm

Data collection

Siemens CCD three-circle diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.537$, $T_{\max} = 0.764$
76 863 measured reflections
10 902 independent reflections
9631 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.023$
$\theta_{\max} = 29.7°$
$h = -24 \rightarrow 22$
$k = -30 \rightarrow 30$
$l = -13 \rightarrow 14$
123 standard reflections
frequency: 1000 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.061$
$S = 1.13$
10 902 reflections
455 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0258P)^2 + 2.4763P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.005$
$\Delta\rho_{\max} = 0.40$ e Å^{-3}
$\Delta\rho_{\min} = -0.78$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

Sn1—O11	2.1233 (13)	Sn1*A*—O11A	2.1268 (14)
Sn1—O21	2.1248 (13)	Sn1*A*—O21*A*	2.1503 (14)
Sn1—O22	2.5553 (14)	Sn1*A*—O12*A*	2.4967 (17)
Sn1—O12	2.5641 (14)	Sn1*A*—O22*A*	2.5407 (16)

The two thiophene rings are disordered. The resolution of the data did not allow for distinguishing two distinct positions for the S and C atoms. Only one peak was found for each atom in the difference map. Thus, a C and an S atom were refined sharing the same position and the same displacement parameters, and just refining the site-occupation factor of the respective C and S atoms in order to determine the ratio of the different orientations, which turned out to be 0.644 (3) for S13 and C16, 0.810 (3) for S23 and C26, 0.760 (3) for S13*A* and C16*A*, and 0.904 (3) for S23*A* and C26*A*. All H atoms were located by difference Fourier synthesis and refined with fixed individual displacement parameters [U(H) = 1.2$U_{\rm eq}$(C) or U(H) = 1.5$U_{\rm eq}$(C$_{\rm methyl}$)] using a riding model with aromatic C—H = 0.95 Å, methyl C—H = 0.98 Å or methylene C—H = 0.99 Å.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

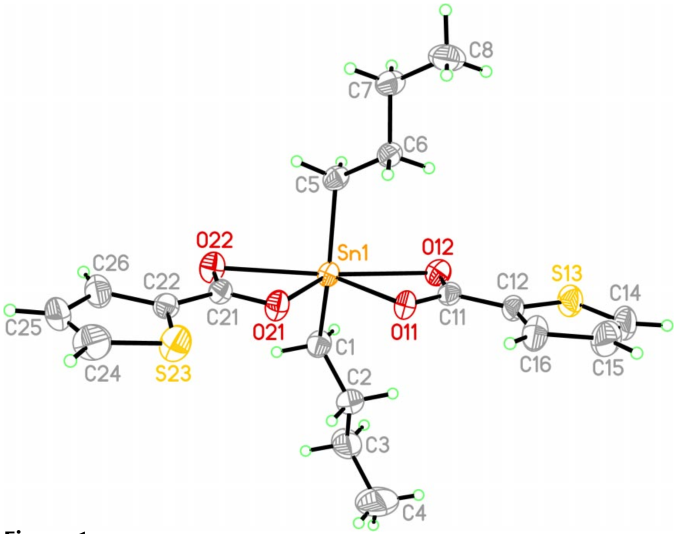


Figure 1
A perspective view of molecule 1 of the title compound with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level.

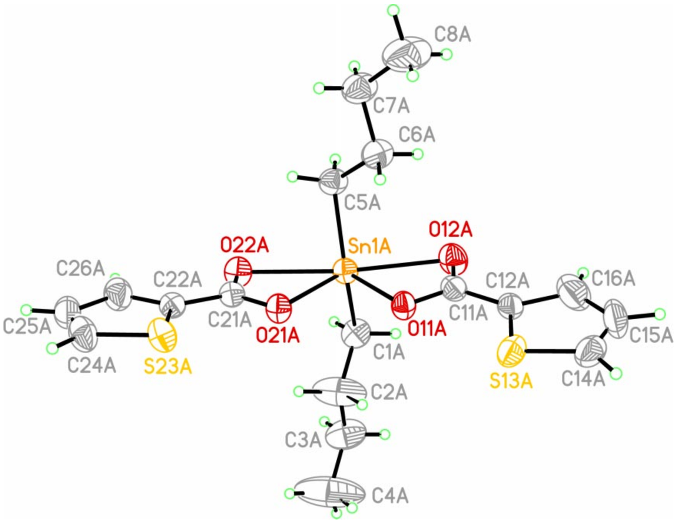


Figure 2
A perspective view of molecule 2 of the title compound with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level.

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