Acta Crystallographica Section C
**Crystal Structure**
**Communications**
ISSN 0108-2701

# Orthorhombic modification of triphenyltin 3-ureidopropionate

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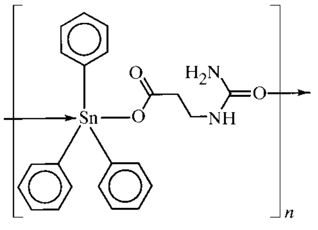
Received 31 January 2000
Accepted 9 February 2000

Data validation number: IUC0000044

The Sn atom in *catena*-poly[triphenyltin(IV)-$\mu$-(3-ureidopropionato-$O^1$:$O^3$)], $[Sn(C_6H_5)_3(C_4H_7N_2O_3)]_n$, is five-coordinate and has a *trans*-$C_3SnO_2$ trigonal-bipyrmidal geometry arising from bridging through the O atom of the ureido fragment of an adjacent carboxylate group. Infinite chains propagate helically along the *c* axis and adjacent chains are linked by N—H···O [N···O 2.851 (4) Å] hydrogen bonds into layers.

## Comment

Triphenyltin alkanoates generally adopt carboxylate-bridged chain structures whose chains have either a flat or a helical conformation (Ng *et al.*, 1988; Tiekink, 1991, 1994). A strongly Lewis-basic site in the alkanoate group can compete successfully with the carboxyl O atom, and this is exemplified by the diethylphosphonoacetate (Ng & Kumar Das, 1994) and 3-diethylphosphonopropionate (Ng & Kumar Das, 1996). The ureido O atom in the 3-ureidopropionate is probably more basic than the phosphoryl O atoms in 3-diethylphosphonopionate [Sn—O 2.116 (2) Å and Sn←O 2.397 (3) Å] as the dative bond [Sn—O = 2.161 (2) Å and Sn←O 2.327 (2) Å] is much shorter than than in the 3-diethylphosphopripionate. Bond dimensions involving the Sn atom in the orthorhombic modification, (I), do not differ much from those found in the monoclinic modification (Lo *et al.*, 1991); the most significant difference is the almost linear O—Sn←O skeleton [O—Sn←O 179.2 (1)°], which contrasts with the bent skeleton [O—Sn←O 171.5 (1)°] of the monoclinic modification. The monoclinic ($P2_1/n$) modification which propagates in a zigzag manner along the *c* axis, adopts a similar hydrogen-bonded [N···O 2.882 (4) Å] architecture.



(I)

## Experimental

The crystal used for the X-ray measurements was a crystal that was selected from a batch of triphenyltin *N*,*N*-3-oxapentamethylenethiocarbamoylthioacetate hydrate (Ng & Hook, 1999) crystals that had been kept in a bottle for several years. Whether the crystal had resulted from the solid-state decomposition of the hydrate or whether 3-ureidopropionic acid was a contaminant in the *N*,*N*-3-oxapentamethylenethiocarbamoylacetic acid that reacted with triphenyltin hydroxide to form the 3-ureidopropionate could not be ascertained.

### *Crystal data*

$[Sn(C_6H_5)_3(C_4H_7N_2O_3)]$
$M_r = 481.11$
Orthorhombic, $P2_12_12_1$
$a = 11.2608\ (6)$ Å
$b = 13.0527\ (5)$ Å
$c = 14.6607\ (6)$ Å
$V = 2154.9\ (2)$ Å$^3$
$Z = 4$
$D_x = 1.483$ Mg m$^{-3}$

Mo *Kα* radiation
Cell parameters from 25 reflections
$\theta = 14.5$–$15.0°$
$\mu = 1.209$ mm$^{-1}$
$T = 298\ (2)$ K
Cube, colorless
0.43 × 0.43 × 0.43 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$ scans
Absorption correction: semi-empirical $\psi$ scans [North *et al.* (1968) in *WinGX* (Farrugia, 1999)]
$T_{min} = 0.6661$, $T_{max} = 0.7239$
7014 measured reflections
6262 independent reflections

5401 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 29.97°$
$h = -15 \rightarrow 15$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 20$
3 standard reflections
frequency: 60 min
intensity decay: 3%

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.077$
$S = 1.056$
6262 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.828$ e Å$^{-3}$
$\Delta\rho_{min} = -0.314$ e Å$^{-3}$
Absolute structure: Flack & Schwarzenbach (1988)
Flack parameter = −0.04 (2); 2752 Friedel pairs

The structure was refined using 6262 reflections (3510 unique and an additional 2752 Friedel pairs); the chirality of the crystal used in the measurements was established by the Flack parameter, which refined to -0.04 (2).

Data collection: *CAD*-4/*PC* (Kretschmar, 1994); cell refinement: *CELDIM* in *CAD*-4 *VAX*/*PC Fortran System* (Enraf–Nonius, 1988); data reduction: *XCAD*4 (Harms, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

I thank the National Science Council for R&D (IRPA 09–02–03–0371) for supporting this work.

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