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## Structure Reports

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# catena-Poly[[triphenyltin(IV)]- $\mu$ -N-(4-acetylphenyl)maleamato]

 Moazzam H. Bhatti,<sup>a\*</sup> Uzma Yunus,<sup>a</sup> Nosheen Mussarat,<sup>a</sup> Madeleine Helliwell<sup>b</sup> and Richard Prendergast<sup>b</sup>
<sup>a</sup>Department of Chemistry, Allama Iqbal Open University, Islamabad, Pakistan, and

<sup>b</sup>School of Chemistry, University of Manchester, Manchester M30 9PL, England

Correspondence e-mail: moazzamhussain\_b@yahoo.com

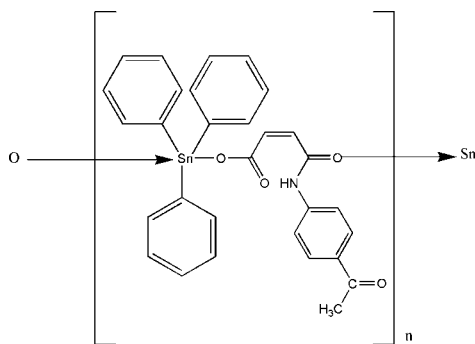
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 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.061; data-to-parameter ratio = 11.8.

The crystal structure of the polymeric title compound,  $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{12}\text{H}_{10}\text{NO}_4)]_n$ , comprises polymeric chains whereby adjacent Sn atoms are bridged by carboxylate and amide carbonyl O atoms [ $\text{Sn}-\text{O} = 2.115$  (15) and 2.653 (1) Å, respectively]. The  $\text{Sn}^{\text{IV}}$  atom is five-coordinated showing a distorted trigonal-bipyramid geometry, with the three phenyl *ipso*-C atoms defining the trigonal plane and the axial positions occupied by O atoms [ $\text{O}-\text{Sn}-\text{O} = 171.91$  (5)°]. Intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonding leads to a seven-membered loop. There is an intramolecular  $\text{C}-\text{H}\cdots\text{O}$  interaction within the polymeric chain. An intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interaction along  $c$  links the polymeric chains into sheets which are linked into a three-dimensional network *via*  $\text{C}-\text{H}\cdots\pi$  interactions.

## Related literature

For reviews of organotin structural chemistry, see: Tiekink (1991, 1994). For related structures, see: Sadiq-ur-Rehman *et al.* (2005); Parvez *et al.* (2002).



## Experimental

## Crystal data

 $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{12}\text{H}_{10}\text{NO}_4)]$ 
 $M_r = 582.20$ 

 Triclinic,  $P\bar{1}$ 
 $a = 9.7556$  (5) Å

 $b = 11.3298$  (6) Å

 $c = 12.0571$  (6) Å

 $\alpha = 73.187$  (1)°

 $\beta = 87.082$  (1)°

 $\gamma = 79.841$  (1)°

 $V = 1255.69$  (11) Å<sup>3</sup>
 $Z = 2$ 

 Mo  $K\alpha$  radiation

 $\mu = 1.05$  mm<sup>-1</sup>
 $T = 100$  K

 $0.40 \times 0.30 \times 0.30$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan

 (*SADABS*; Bruker, 2001)

 $T_{\text{min}} = 0.726$ ,  $T_{\text{max}} = 1.000$ 

10025 measured reflections

5034 independent reflections

 4905 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.017$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.024$ 
 $wR(F^2) = 0.061$ 
 $S = 1.09$ 

5034 reflections

425 parameters

All H-atom parameters refined

 $\Delta\rho_{\text{max}} = 0.94$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.52$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

 $\text{Cg1}-\text{Cg3}$  are the centroids of the C1–C6, C7–C12 and C13–C18 benzene rings, respectively.

| $D-\text{H}\cdots A$                                | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1N}\cdots\text{O2}$               | 0.87 (3)     | 1.88 (3)           | 2.707 (2)   | 158 (2)              |
| $\text{C6}-\text{H6}\cdots\text{O3}^{\text{i}}$     | 0.91 (3)     | 2.58 (3)           | 3.253 (3)   | 131 (2)              |
| $\text{C20}-\text{H20}\cdots\text{O4}^{\text{ii}}$  | 0.93 (3)     | 2.48 (3)           | 3.242 (3)   | 139 (2)              |
| $\text{C3}-\text{H3}\cdots\text{Cg2}^{\text{iii}}$  | 0.92 (3)     | 2.93 (3)           | 3.651 (2)   | 137 (2)              |
| $\text{C27}-\text{H27}\cdots\text{Cg3}^{\text{iv}}$ | 0.92 (3)     | 2.83 (3)           | 3.674 (2)   | 154 (2)              |
| $\text{C30}-\text{H30C}\cdots\text{Cg1}^{\text{v}}$ | 0.93 (3)     | 2.93 (3)           | 3.794 (4)   | 155 (3)              |

 Symmetry codes: (i)  $x+1, y, z$ ; (ii)  $x, y, z+1$ ; (iii)  $-x+2, -y, -z+1$ ; (iv)  $-x+2, -y+1, -z$ ; (v)  $x-1, y, z-1$ .

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5234).

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## supporting information

*Acta Cryst.* (2013). E69, m427 [doi:10.1107/S1600536813017613]

**catena-Poly[[triphenyltin(IV)]- $\mu$ -N-(4-acetylphenyl)maleamato]**

**Moazzam H. Bhatti, Uzma Yunus, Nosheen Mussarat, Madeleine Helliwell and Richard Prendergast**

**S1. Comment**

Organotin(IV) carboxylates are well known for their potential applications and rich structural diversity (Tiekink, 1991). Among organotin(IV) carboxylates, tri-organotin(IV) carboxylates have shown discrete to polymer chain structures (Tiekink, 1994). Triphenyltin(IV) carboxylates generally adopt a tetrahedral geometry with a monodentate carboxylate [Sadiq-ur-Rehman *et al.*, 2005] or a distorted trigonal bipyramidal geometry with bridging ligand or with an additional donor atom like N or O derived from the adjacent ligand [Parvez *et al.*, 2002]. In the present report we have studied the polymeric title compound, (I), *catena*-poly{[triphenyltin(IV)]- $\mu$ -N-(4-acetylphenyl)maleamato}, (Fig. 1).

The geometry around tin atom is distorted trigonal bipyramidal as defined by three *ipso*-carbon atoms of the three phenyl rings in equatorial positions [Sn1—C1 = 2.133 (2) Å, Sn1—C7 = 2.117 (2) Å, Sn1—C13 = 2.119 (2) Å] while the axial positions are occupied by the O atom of a monodentate carboxylate ligand [Sn1—O1 = 2.115 (15) Å] and the amide carbonyl of an adjacent ligand [Sn1—O3 = 2.653 (1) Å]. The sum of the angles in the equatorial plane is 354.9° indicating distortion. The major distortion from ideal trigonal bipyramidal geometry is found in the axial angle [O1—Sn1—O3 = 171.91 (5)°]. The monodentate mode of coordination of the carboxylate ligand is reflected in the disparate O1—C19 and O2—C19 bond distances of 1.295 (3) and 1.234 (3) Å, respectively, with the longer separation associated with the stronger Sn1—O1 interaction. The much longer distance, Sn1—O2 = 3.100 (1) Å, further demonstrates the monodentate nature of the carboxylate ligand. Although this value is quite long for any coordination of Sn with O, it falls well within the sum of their van der Waals radii (3.70 Å). Adjacent Sn atoms are linked by the O1 and O3 atoms of each ligand generating polymeric chains (Fig. 2).

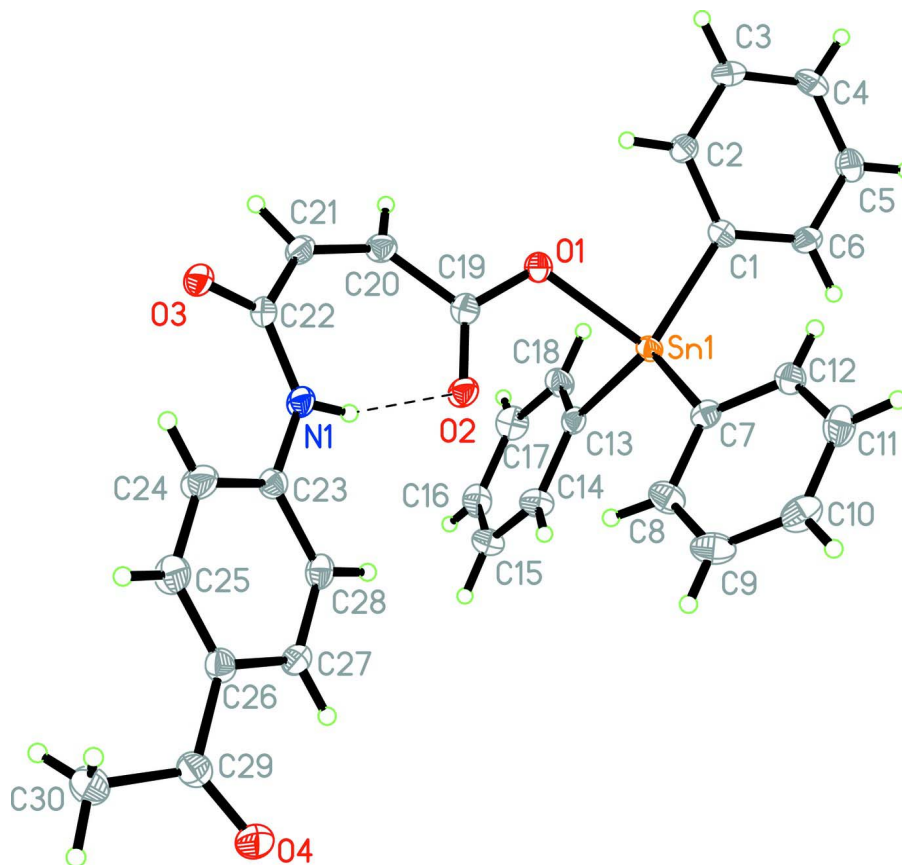
The ligand forms an essentially planar seven-membered ring involving an intramolecular N1—H1N $\cdots$ O2 hydrogen bond (Figs 1 and 2).

**S2. Experimental**

A solution of maleic anhydride (1.0 g, 10 mmol) in ethyl acetate (50 ml) was added to a solution of *p*-aminoacetophenone (1.35 g, 10 mmol) in ethyl acetate (50 ml) in a 250 ml conical flask. The mixture was stirred for 3 h at room temperature. After stirring, the precipitates of the acid were filtered and recrystallized with ethanol. Equimolar amounts of acid (2.33 g, 10 mmol) and triphenyltin hydroxide (3.17 g 10.0 mmol) were suspended in a dry ethanol / acetone (100 ml, 8:2) solvent mixture and refluxed for 8 h. After cooling to room temperature, the reaction mixture was filtered and solvents were evaporated in rotary evaporator. The solid obtained was recrystallized from chloroform with few drops of *n*-hexane.

## S3. Refinement

H atoms were found by difference Fourier techniques and refined isotropically.



**Figure 1**

The asymmetric unit of (I) with atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

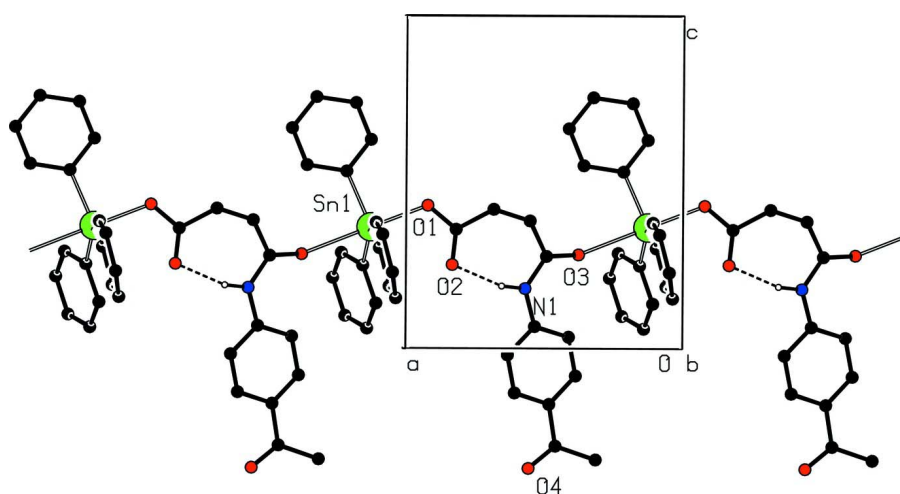


Figure 2

Polymeric chains viewed down *b*. The intramolecular N1—H1N···O2 hydrogen bonds are shown with dashed lines.

**catena-Poly[[triphenyltin(IV)]- $\mu$ -*N*-(4-acetylphenyl)maleamato]**

*Crystal data*

[Sn(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>(C<sub>12</sub>H<sub>10</sub>NO<sub>4</sub>)]

$M_r = 582.20$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 9.7556$  (5) Å

$b = 11.3298$  (6) Å

$c = 12.0571$  (6) Å

$\alpha = 73.187$  (1)°

$\beta = 87.082$  (1)°

$\gamma = 79.841$  (1)°

$V = 1255.69$  (11) Å<sup>3</sup>

$Z = 2$

$F(000) = 588$

$D_x = 1.540$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 7807 reflections

$\theta = 2.2$ – $26.3$ °

$\mu = 1.05$  mm<sup>-1</sup>

$T = 100$  K

Block, colourless

0.40 × 0.30 × 0.30 mm

*Data collection*

Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.726$ ,  $T_{\max} = 1.000$

10025 measured reflections

5034 independent reflections

4905 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\max} = 26.4$ °,  $\theta_{\min} = 1.9$ °

$h = -12$ → $12$

$k = -14$ → $14$

$l = -14$ → $14$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.061$

$S = 1.09$

5034 reflections

425 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.7706P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.94$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.52$  e Å<sup>-3</sup>

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)*

|     | <i>x</i>      | <i>y</i>      | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|---------------|----------------------------------|
| Sn1 | 1.118867 (13) | 0.216792 (11) | 0.364576 (10) | 0.01473 (6)                      |

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|     |              |              |               |            |
|-----|--------------|--------------|---------------|------------|
| O1  | 0.91398 (14) | 0.21171 (14) | 0.43008 (12)  | 0.0192 (3) |
| O2  | 0.82580 (15) | 0.29679 (14) | 0.25203 (12)  | 0.0203 (3) |
| O3  | 0.36940 (15) | 0.25668 (14) | 0.28265 (12)  | 0.0207 (3) |
| O4  | 0.54744 (17) | 0.37815 (17) | -0.35968 (13) | 0.0294 (4) |
| N1  | 0.56244 (18) | 0.31413 (16) | 0.18064 (15)  | 0.0180 (3) |
| C1  | 1.2068 (2)   | 0.12405 (18) | 0.53210 (17)  | 0.0157 (4) |
| C2  | 1.1190 (2)   | 0.09341 (19) | 0.62727 (18)  | 0.0188 (4) |
| C3  | 1.1730 (2)   | 0.0327 (2)   | 0.73784 (18)  | 0.0223 (4) |
| C4  | 1.3154 (2)   | 0.0025 (2)   | 0.75508 (18)  | 0.0229 (4) |
| C5  | 1.4035 (2)   | 0.0305 (2)   | 0.6616 (2)    | 0.0249 (5) |
| C6  | 1.3499 (2)   | 0.0898 (2)   | 0.55069 (19)  | 0.0214 (4) |
| C7  | 1.1471 (2)   | 0.10390 (19) | 0.24991 (17)  | 0.0163 (4) |
| C8  | 1.0993 (2)   | 0.1477 (2)   | 0.13559 (19)  | 0.0228 (4) |
| C9  | 1.1310 (3)   | 0.0744 (2)   | 0.0605 (2)    | 0.0261 (5) |
| C10 | 1.2088 (2)   | -0.0445 (2)  | 0.0984 (2)    | 0.0256 (5) |
| C11 | 1.2536 (2)   | -0.0907 (2)  | 0.2129 (2)    | 0.0246 (5) |
| C12 | 1.2232 (2)   | -0.0165 (2)  | 0.28751 (19)  | 0.0199 (4) |
| C13 | 1.0903 (2)   | 0.41459 (18) | 0.30166 (17)  | 0.0163 (4) |
| C14 | 1.0550 (2)   | 0.4792 (2)   | 0.18678 (19)  | 0.0227 (4) |
| C15 | 1.0324 (2)   | 0.6089 (2)   | 0.15076 (19)  | 0.0246 (5) |
| C16 | 1.0452 (2)   | 0.6755 (2)   | 0.2282 (2)    | 0.0239 (4) |
| C17 | 1.0806 (2)   | 0.6130 (2)   | 0.3421 (2)    | 0.0248 (5) |
| C18 | 1.1028 (2)   | 0.4831 (2)   | 0.37833 (19)  | 0.0210 (4) |
| C19 | 0.8119 (2)   | 0.26463 (19) | 0.35832 (18)  | 0.0176 (4) |
| C20 | 0.6763 (2)   | 0.2894 (2)   | 0.41850 (18)  | 0.0195 (4) |
| C21 | 0.5453 (2)   | 0.3011 (2)   | 0.38405 (18)  | 0.0190 (4) |
| C22 | 0.4852 (2)   | 0.28728 (18) | 0.27760 (17)  | 0.0172 (4) |
| C23 | 0.5275 (2)   | 0.32237 (19) | 0.06658 (17)  | 0.0172 (4) |
| C24 | 0.4041 (2)   | 0.2941 (2)   | 0.0351 (2)    | 0.0259 (5) |
| C25 | 0.3785 (2)   | 0.3122 (2)   | -0.0815 (2)   | 0.0258 (5) |
| C26 | 0.4739 (2)   | 0.35404 (19) | -0.16698 (18) | 0.0193 (4) |
| C27 | 0.5990 (2)   | 0.3783 (2)   | -0.13311 (18) | 0.0195 (4) |
| C28 | 0.6248 (2)   | 0.36391 (19) | -0.01899 (19) | 0.0194 (4) |
| C29 | 0.4505 (2)   | 0.3716 (2)   | -0.29234 (18) | 0.0218 (4) |
| C30 | 0.3051 (3)   | 0.3806 (3)   | -0.3335 (2)   | 0.0289 (5) |
| H2  | 1.023 (3)    | 0.112 (2)    | 0.618 (2)     | 0.023 (6)* |
| H3  | 1.112 (3)    | 0.013 (3)    | 0.798 (2)     | 0.032 (7)* |
| H4  | 1.354 (3)    | -0.036 (3)   | 0.826 (3)     | 0.033 (7)* |
| H5  | 1.498 (3)    | 0.004 (3)    | 0.672 (2)     | 0.032 (7)* |
| H6  | 1.409 (3)    | 0.107 (2)    | 0.489 (2)     | 0.027 (7)* |
| H8  | 1.047 (3)    | 0.227 (3)    | 0.113 (2)     | 0.024 (6)* |
| H9  | 1.104 (3)    | 0.105 (3)    | -0.011 (3)    | 0.042 (8)* |
| H10 | 1.228 (3)    | -0.092 (3)   | 0.049 (2)     | 0.031 (7)* |
| H11 | 1.304 (3)    | -0.170 (3)   | 0.240 (2)     | 0.026 (7)* |
| H12 | 1.254 (3)    | -0.046 (2)   | 0.357 (2)     | 0.020 (6)* |
| H14 | 1.045 (3)    | 0.436 (3)    | 0.132 (2)     | 0.030 (7)* |
| H15 | 1.010 (3)    | 0.650 (3)    | 0.075 (2)     | 0.030 (7)* |
| H16 | 1.032 (3)    | 0.756 (2)    | 0.206 (2)     | 0.020 (6)* |

|      |           |           |            |            |
|------|-----------|-----------|------------|------------|
| H17  | 1.085 (3) | 0.654 (3) | 0.393 (2)  | 0.030 (7)* |
| H18  | 1.127 (3) | 0.442 (2) | 0.453 (2)  | 0.026 (6)* |
| H20  | 0.688 (3) | 0.302 (2) | 0.489 (2)  | 0.021 (6)* |
| H21  | 0.476 (3) | 0.319 (2) | 0.437 (2)  | 0.022 (6)* |
| H24  | 0.339 (3) | 0.263 (3) | 0.091 (3)  | 0.036 (7)* |
| H25  | 0.301 (3) | 0.293 (3) | -0.103 (2) | 0.037 (8)* |
| H27  | 0.663 (3) | 0.408 (3) | -0.188 (2) | 0.032 (7)* |
| H28  | 0.711 (3) | 0.385 (3) | 0.001 (2)  | 0.031 (7)* |
| H30A | 0.303 (3) | 0.410 (3) | -0.412 (3) | 0.045 (8)* |
| H30B | 0.244 (3) | 0.434 (3) | -0.300 (2) | 0.027 (7)* |
| H30C | 0.282 (3) | 0.301 (3) | -0.315 (3) | 0.037 (8)* |
| H1N  | 0.647 (3) | 0.326 (2) | 0.188 (2)  | 0.025 (7)* |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Sn1 | 0.01521 (8) | 0.01594 (8) | 0.01313 (8) | -0.00281 (5) | -0.00159 (5) | -0.00392 (5) |
| O1  | 0.0137 (7)  | 0.0241 (7)  | 0.0190 (7)  | -0.0039 (6)  | -0.0019 (5)  | -0.0040 (6)  |
| O2  | 0.0153 (7)  | 0.0291 (8)  | 0.0178 (7)  | -0.0057 (6)  | 0.0007 (5)   | -0.0075 (6)  |
| O3  | 0.0140 (7)  | 0.0280 (8)  | 0.0195 (7)  | -0.0051 (6)  | 0.0003 (5)   | -0.0052 (6)  |
| O4  | 0.0261 (8)  | 0.0426 (10) | 0.0191 (8)  | -0.0003 (7)  | 0.0007 (6)   | -0.0114 (7)  |
| N1  | 0.0129 (8)  | 0.0242 (9)  | 0.0178 (8)  | -0.0044 (7)  | -0.0005 (6)  | -0.0067 (7)  |
| C1  | 0.0183 (10) | 0.0133 (9)  | 0.0165 (9)  | -0.0044 (7)  | -0.0015 (7)  | -0.0044 (7)  |
| C2  | 0.0162 (10) | 0.0197 (10) | 0.0203 (10) | -0.0049 (8)  | 0.0007 (8)   | -0.0045 (8)  |
| C3  | 0.0267 (11) | 0.0232 (11) | 0.0164 (10) | -0.0081 (9)  | 0.0048 (8)   | -0.0032 (8)  |
| C4  | 0.0299 (12) | 0.0211 (10) | 0.0151 (10) | -0.0025 (9)  | -0.0057 (8)  | -0.0010 (8)  |
| C5  | 0.0172 (11) | 0.0305 (12) | 0.0247 (11) | -0.0021 (9)  | -0.0055 (8)  | -0.0046 (9)  |
| C6  | 0.0182 (10) | 0.0252 (11) | 0.0191 (10) | -0.0057 (8)  | 0.0032 (8)   | -0.0031 (8)  |
| C7  | 0.0147 (9)  | 0.0191 (10) | 0.0173 (9)  | -0.0069 (7)  | 0.0013 (7)   | -0.0064 (8)  |
| C8  | 0.0291 (11) | 0.0179 (10) | 0.0210 (10) | -0.0053 (9)  | -0.0030 (9)  | -0.0037 (8)  |
| C9  | 0.0374 (13) | 0.0270 (11) | 0.0174 (11) | -0.0131 (10) | -0.0009 (9)  | -0.0072 (9)  |
| C10 | 0.0305 (12) | 0.0261 (11) | 0.0266 (11) | -0.0110 (9)  | 0.0071 (9)   | -0.0150 (10) |
| C11 | 0.0212 (11) | 0.0204 (11) | 0.0337 (12) | -0.0028 (9)  | 0.0012 (9)   | -0.0106 (9)  |
| C12 | 0.0163 (10) | 0.0227 (11) | 0.0204 (11) | -0.0050 (8)  | -0.0016 (8)  | -0.0043 (8)  |
| C13 | 0.0124 (9)  | 0.0170 (9)  | 0.0192 (10) | -0.0032 (7)  | 0.0009 (7)   | -0.0044 (8)  |
| C14 | 0.0280 (11) | 0.0222 (11) | 0.0183 (10) | -0.0059 (9)  | -0.0001 (8)  | -0.0055 (8)  |
| C15 | 0.0273 (11) | 0.0231 (11) | 0.0194 (11) | -0.0036 (9)  | 0.0000 (9)   | -0.0001 (9)  |
| C16 | 0.0217 (11) | 0.0169 (11) | 0.0320 (12) | -0.0046 (8)  | 0.0009 (9)   | -0.0047 (9)  |
| C17 | 0.0263 (11) | 0.0247 (11) | 0.0282 (12) | -0.0074 (9)  | -0.0019 (9)  | -0.0127 (9)  |
| C18 | 0.0204 (10) | 0.0238 (11) | 0.0188 (10) | -0.0034 (8)  | -0.0042 (8)  | -0.0056 (8)  |
| C19 | 0.0160 (9)  | 0.0189 (10) | 0.0200 (10) | -0.0051 (8)  | -0.0015 (8)  | -0.0074 (8)  |
| C20 | 0.0202 (10) | 0.0229 (10) | 0.0163 (10) | -0.0048 (8)  | 0.0004 (8)   | -0.0062 (8)  |
| C21 | 0.0172 (10) | 0.0228 (10) | 0.0175 (10) | -0.0034 (8)  | 0.0034 (8)   | -0.0069 (8)  |
| C22 | 0.0144 (9)  | 0.0174 (9)  | 0.0183 (10) | 0.0000 (7)   | -0.0001 (7)  | -0.0044 (8)  |
| C23 | 0.0157 (9)  | 0.0196 (10) | 0.0167 (9)  | -0.0023 (8)  | -0.0008 (7)  | -0.0061 (8)  |
| C24 | 0.0189 (10) | 0.0395 (13) | 0.0211 (11) | -0.0116 (9)  | 0.0017 (8)   | -0.0080 (10) |
| C25 | 0.0173 (10) | 0.0388 (13) | 0.0250 (11) | -0.0103 (9)  | -0.0032 (8)  | -0.0107 (10) |
| C26 | 0.0183 (10) | 0.0199 (10) | 0.0199 (10) | -0.0009 (8)  | -0.0015 (8)  | -0.0073 (8)  |

|     |             |             |             |              |             |              |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C27 | 0.0160 (10) | 0.0237 (10) | 0.0186 (10) | -0.0026 (8)  | 0.0024 (8)  | -0.0065 (8)  |
| C28 | 0.0136 (9)  | 0.0215 (10) | 0.0240 (11) | -0.0046 (8)  | -0.0007 (8) | -0.0069 (8)  |
| C29 | 0.0247 (11) | 0.0210 (10) | 0.0200 (10) | -0.0001 (8)  | -0.0023 (8) | -0.0079 (8)  |
| C30 | 0.0264 (12) | 0.0409 (14) | 0.0217 (12) | -0.0038 (10) | -0.0046 (9) | -0.0130 (11) |

*Geometric parameters (Å, °)*

|            |             |             |            |
|------------|-------------|-------------|------------|
| Sn1—O1     | 2.1156 (14) | C12—H12     | 0.85 (3)   |
| Sn1—C7     | 2.117 (2)   | C13—C18     | 1.390 (3)  |
| Sn1—C13    | 2.120 (2)   | C13—C14     | 1.395 (3)  |
| Sn1—C1     | 2.1331 (19) | C14—C15     | 1.387 (3)  |
| O1—C19     | 1.295 (2)   | C14—H14     | 0.95 (3)   |
| O2—C19     | 1.234 (3)   | C15—C16     | 1.382 (3)  |
| O3—C22     | 1.233 (2)   | C15—H15     | 0.92 (3)   |
| O4—C29     | 1.213 (3)   | C16—C17     | 1.380 (3)  |
| N1—C22     | 1.346 (3)   | C16—H16     | 0.86 (3)   |
| N1—C23     | 1.406 (3)   | C17—C18     | 1.388 (3)  |
| N1—H1N     | 0.87 (3)    | C17—H17     | 0.88 (3)   |
| C1—C6      | 1.394 (3)   | C18—H18     | 0.91 (3)   |
| C1—C2      | 1.395 (3)   | C19—C20     | 1.498 (3)  |
| C2—C3      | 1.393 (3)   | C20—C21     | 1.336 (3)  |
| C2—H2      | 0.93 (3)    | C20—H20     | 0.93 (3)   |
| C3—C4      | 1.382 (3)   | C21—C22     | 1.497 (3)  |
| C3—H3      | 0.92 (3)    | C21—H21     | 0.94 (3)   |
| C4—C5      | 1.379 (3)   | C23—C24     | 1.396 (3)  |
| C4—H4      | 0.90 (3)    | C23—C28     | 1.401 (3)  |
| C5—C6      | 1.393 (3)   | C24—C25     | 1.390 (3)  |
| C5—H5      | 0.92 (3)    | C24—H24     | 0.94 (3)   |
| C6—H6      | 0.91 (3)    | C25—C26     | 1.388 (3)  |
| C7—C12     | 1.392 (3)   | C25—H25     | 0.89 (3)   |
| C7—C8      | 1.397 (3)   | C26—C27     | 1.402 (3)  |
| C8—C9      | 1.386 (3)   | C26—C29     | 1.490 (3)  |
| C8—H8      | 0.92 (3)    | C27—C28     | 1.369 (3)  |
| C9—C10     | 1.385 (3)   | C27—H27     | 0.92 (3)   |
| C9—H9      | 0.87 (3)    | C28—H28     | 0.97 (3)   |
| C10—C11    | 1.390 (3)   | C29—C30     | 1.504 (3)  |
| C10—H10    | 0.90 (3)    | C30—H30A    | 0.90 (3)   |
| C11—C12    | 1.388 (3)   | C30—H30B    | 0.93 (3)   |
| C11—H11    | 0.91 (3)    | C30—H30C    | 0.93 (3)   |
| O1—Sn1—C7  | 106.04 (6)  | C16—C15—C14 | 120.3 (2)  |
| O1—Sn1—C13 | 94.72 (6)   | C16—C15—H15 | 120.2 (17) |
| C7—Sn1—C13 | 121.26 (8)  | C14—C15—H15 | 119.4 (17) |
| O1—Sn1—C1  | 91.79 (7)   | C17—C16—C15 | 120.0 (2)  |
| C7—Sn1—C1  | 113.71 (7)  | C17—C16—H16 | 119.3 (16) |
| C13—Sn1—C1 | 119.95 (7)  | C15—C16—H16 | 120.7 (16) |
| C19—O1—Sn1 | 117.65 (13) | C16—C17—C18 | 119.7 (2)  |
| C22—N1—C23 | 128.88 (18) | C16—C17—H17 | 121.0 (18) |

|                |             |                 |             |
|----------------|-------------|-----------------|-------------|
| C22—N1—H1N     | 117.3 (17)  | C18—C17—H17     | 119.2 (18)  |
| C23—N1—H1N     | 113.8 (17)  | C17—C18—C13     | 121.1 (2)   |
| C6—C1—C2       | 117.95 (19) | C17—C18—H18     | 119.7 (17)  |
| C6—C1—Sn1      | 122.54 (15) | C13—C18—H18     | 119.3 (17)  |
| C2—C1—Sn1      | 119.49 (15) | O2—C19—O1       | 123.74 (19) |
| C3—C2—C1       | 120.93 (19) | O2—C19—C20      | 123.54 (18) |
| C3—C2—H2       | 118.3 (16)  | O1—C19—C20      | 112.62 (17) |
| C1—C2—H2       | 120.8 (16)  | C21—C20—C19     | 130.75 (19) |
| C4—C3—C2       | 120.3 (2)   | C21—C20—H20     | 116.9 (15)  |
| C4—C3—H3       | 121.6 (17)  | C19—C20—H20     | 112.3 (15)  |
| C2—C3—H3       | 118.2 (17)  | C20—C21—C22     | 132.41 (19) |
| C5—C4—C3       | 119.4 (2)   | C20—C21—H21     | 115.4 (15)  |
| C5—C4—H4       | 118.2 (18)  | C22—C21—H21     | 112.2 (15)  |
| C3—C4—H4       | 122.3 (18)  | O3—C22—N1       | 124.60 (19) |
| C4—C5—C6       | 120.5 (2)   | O3—C22—C21      | 119.31 (18) |
| C4—C5—H5       | 119.5 (17)  | N1—C22—C21      | 116.05 (18) |
| C6—C5—H5       | 119.9 (17)  | C24—C23—C28     | 119.58 (19) |
| C5—C6—C1       | 120.9 (2)   | C24—C23—N1      | 124.44 (19) |
| C5—C6—H6       | 119.6 (17)  | C28—C23—N1      | 115.97 (18) |
| C1—C6—H6       | 119.5 (17)  | C25—C24—C23     | 118.9 (2)   |
| C12—C7—C8      | 118.41 (19) | C25—C24—H24     | 119.9 (18)  |
| C12—C7—Sn1     | 118.82 (15) | C23—C24—H24     | 121.2 (18)  |
| C8—C7—Sn1      | 122.66 (15) | C26—C25—C24     | 121.9 (2)   |
| C9—C8—C7       | 120.7 (2)   | C26—C25—H25     | 118.3 (19)  |
| C9—C8—H8       | 122.1 (16)  | C24—C25—H25     | 119.8 (19)  |
| C7—C8—H8       | 117.2 (16)  | C25—C26—C27     | 118.27 (19) |
| C10—C9—C8      | 120.4 (2)   | C25—C26—C29     | 122.99 (19) |
| C10—C9—H9      | 120 (2)     | C27—C26—C29     | 118.72 (19) |
| C8—C9—H9       | 119 (2)     | C28—C27—C26     | 120.75 (19) |
| C9—C10—C11     | 119.6 (2)   | C28—C27—H27     | 118.6 (17)  |
| C9—C10—H10     | 119.5 (18)  | C26—C27—H27     | 120.6 (17)  |
| C11—C10—H10    | 120.9 (18)  | C27—C28—C23     | 120.56 (19) |
| C12—C11—C10    | 119.9 (2)   | C27—C28—H28     | 118.7 (16)  |
| C12—C11—H11    | 119.1 (16)  | C23—C28—H28     | 120.7 (16)  |
| C10—C11—H11    | 121.0 (16)  | O4—C29—C26      | 120.4 (2)   |
| C11—C12—C7     | 121.0 (2)   | O4—C29—C30      | 120.8 (2)   |
| C11—C12—H12    | 118.1 (17)  | C26—C29—C30     | 118.85 (19) |
| C7—C12—H12     | 120.9 (17)  | C29—C30—H30A    | 109 (2)     |
| C18—C13—C14    | 118.53 (19) | C29—C30—H30B    | 108.8 (16)  |
| C18—C13—Sn1    | 118.94 (15) | H30A—C30—H30B   | 111 (3)     |
| C14—C13—Sn1    | 122.50 (15) | C29—C30—H30C    | 109.3 (18)  |
| C15—C14—C13    | 120.3 (2)   | H30A—C30—H30C   | 107 (3)     |
| C15—C14—H14    | 118.4 (16)  | H30B—C30—H30C   | 112 (2)     |
| C13—C14—H14    | 121.2 (16)  |                 |             |
| C7—Sn1—O1—C19  | -67.36 (15) | C7—Sn1—C13—C14  | 16.1 (2)    |
| C13—Sn1—O1—C19 | 57.08 (15)  | C1—Sn1—C13—C14  | 169.33 (16) |
| C1—Sn1—O1—C19  | 177.32 (14) | C18—C13—C14—C15 | -0.3 (3)    |



|                |              |                 |              |
|----------------|--------------|-----------------|--------------|
| O1—Sn1—C1—C6   | 176.43 (17)  | Sn1—C13—C14—C15 | 177.59 (16)  |
| C7—Sn1—C1—C6   | 68.03 (18)   | C13—C14—C15—C16 | 0.3 (3)      |
| C13—Sn1—C1—C6  | -87.08 (18)  | C14—C15—C16—C17 | 0.0 (3)      |
| O1—Sn1—C1—C2   | -2.16 (16)   | C15—C16—C17—C18 | -0.2 (3)     |
| C7—Sn1—C1—C2   | -110.56 (16) | C16—C17—C18—C13 | 0.2 (3)      |
| C13—Sn1—C1—C2  | 94.33 (16)   | C14—C13—C18—C17 | 0.1 (3)      |
| C6—C1—C2—C3    | 1.3 (3)      | Sn1—C13—C18—C17 | -177.87 (16) |
| Sn1—C1—C2—C3   | 179.92 (16)  | Sn1—O1—C19—O2   | 13.9 (3)     |
| C1—C2—C3—C4    | 0.5 (3)      | Sn1—O1—C19—C20  | -162.73 (13) |
| C2—C3—C4—C5    | -1.4 (3)     | O2—C19—C20—C21  | 29.0 (4)     |
| C3—C4—C5—C6    | 0.6 (3)      | O1—C19—C20—C21  | -154.3 (2)   |
| C4—C5—C6—C1    | 1.1 (3)      | C19—C20—C21—C22 | 3.8 (4)      |
| C2—C1—C6—C5    | -2.1 (3)     | C23—N1—C22—O3   | 5.0 (3)      |
| Sn1—C1—C6—C5   | 179.34 (17)  | C23—N1—C22—C21  | -172.72 (19) |
| O1—Sn1—C7—C12  | -102.06 (16) | C20—C21—C22—O3  | 153.0 (2)    |
| C13—Sn1—C7—C12 | 152.00 (15)  | C20—C21—C22—N1  | -29.2 (3)    |
| C1—Sn1—C7—C12  | -2.74 (18)   | C22—N1—C23—C24  | -4.9 (3)     |
| O1—Sn1—C7—C8   | 81.76 (17)   | C22—N1—C23—C28  | 174.1 (2)    |
| C13—Sn1—C7—C8  | -24.2 (2)    | C28—C23—C24—C25 | -2.2 (3)     |
| C1—Sn1—C7—C8   | -178.92 (16) | N1—C23—C24—C25  | 176.7 (2)    |
| C12—C7—C8—C9   | -2.1 (3)     | C23—C24—C25—C26 | 1.9 (4)      |
| Sn1—C7—C8—C9   | 174.13 (17)  | C24—C25—C26—C27 | 0.0 (3)      |
| C7—C8—C9—C10   | 1.0 (3)      | C24—C25—C26—C29 | 178.7 (2)    |
| C8—C9—C10—C11  | 0.8 (3)      | C25—C26—C27—C28 | -1.5 (3)     |
| C9—C10—C11—C12 | -1.7 (3)     | C29—C26—C27—C28 | 179.74 (19)  |
| C10—C11—C12—C7 | 0.6 (3)      | C26—C27—C28—C23 | 1.2 (3)      |
| C8—C7—C12—C11  | 1.2 (3)      | C24—C23—C28—C27 | 0.7 (3)      |
| Sn1—C7—C12—C11 | -175.11 (16) | N1—C23—C28—C27  | -178.29 (19) |
| O1—Sn1—C13—C18 | 82.01 (16)   | C25—C26—C29—O4  | -161.8 (2)   |
| C7—Sn1—C13—C18 | -166.00 (15) | C27—C26—C29—O4  | 16.8 (3)     |
| C1—Sn1—C13—C18 | -12.79 (19)  | C25—C26—C29—C30 | 17.9 (3)     |
| O1—Sn1—C13—C14 | -95.87 (17)  | C27—C26—C29—C30 | -163.4 (2)   |

Hydrogen-bond geometry (Å, °)

Cg1—Cg3 are the centroids of the C1—C6, C7—C12 and C13—C18 benzene rings, respectively.

| <i>D</i> —H... <i>A</i>     | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| N1—H1N...O2                 | 0.87 (3)    | 1.88 (3)      | 2.707 (2)             | 158 (2)                 |
| C6—H6...O3 <sup>i</sup>     | 0.91 (3)    | 2.58 (3)      | 3.253 (3)             | 131 (2)                 |
| C20—H20...O4 <sup>ii</sup>  | 0.93 (3)    | 2.48 (3)      | 3.242 (3)             | 139 (2)                 |
| C3—H3...Cg2 <sup>iii</sup>  | 0.92 (3)    | 2.93 (3)      | 3.651 (2)             | 137 (2)                 |
| C27—H27...Cg3 <sup>iv</sup> | 0.92 (3)    | 2.83 (3)      | 3.674 (2)             | 154 (2)                 |
| C30—H30C...Cg1 <sup>v</sup> | 0.93 (3)    | 2.93 (3)      | 3.794 (4)             | 155 (3)                 |

Symmetry codes: (i)  $x+1, y, z$ ; (ii)  $x, y, z+1$ ; (iii)  $-x+2, -y, -z+1$ ; (iv)  $-x+2, -y+1, -z$ ; (v)  $x-1, y, z-1$ .