Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Octamethyldi-$\mu_3$-oxido-bis($\mu_2$-thiophene-3-acetato-$\kappa^2O$:$O'$)(thiophene-3-acetato-$\kappa O$)tetratin(IV)

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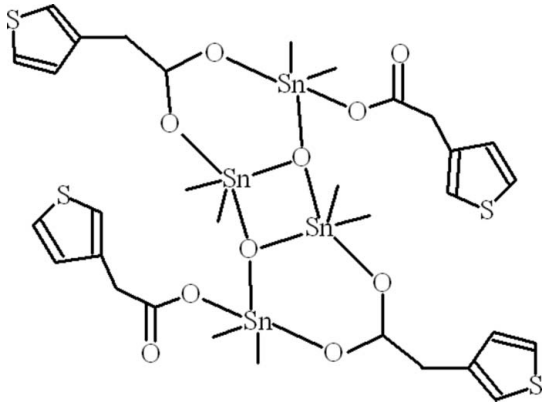
Received 15 April 2009; accepted 25 April 2009

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.006 Å; disorder in main residue; $R$ factor = 0.024; $wR$ factor = 0.059; data-to-parameter ratio = 16.0.

In the centrosymmetric title compound, $[Sn_4(CH_3)_8(C_6H_5O_2S)_4O_2]$, the central four-membered planar ring ($Sn_2O_2$) makes dihedral angles of 66.28 (12) and 77.43 (11)° with the heterocyclic rings of the bridging and monodentate ligands, respectively. One $Sn^{IV}$ atom adopts a distorted $SnO_3C_2$ trigonal-bipyramidal geometry, with both C atoms in equatorial sites and the other a grossly distorted $SnO_4C_2$ octahedral or irregular arrangement. In the crystal, the molecules are connected into pillar-like polymeric units making $R_2^2(12)$ ring motifs due to intermolecular C—H···O interactions. C–H···$\pi$ interactions are also present. The O atoms of the chelating ligands and the S atom of the monodentate ligand are disordered over two sets of sites in a 0.65 (6):0.35 (6) ratio

## Related literature

For related structures, see: Danish *et al.* (1995, 1996); Ng *et al.* (2001); Tahir *et al.* (1997*a*,*b*). For graph-set theory, see: Bernstein *et al.* (1995).



## Experimental

### Crystal data

$[Sn_4(CH_3)_8(C_6H_5O_2S)_4O_2]$
$M_r$ = 1191.79
Triclinic, $P\overline{1}$
$a$ = 9.7330 (5) Å
$b$ = 9.7403 (5) Å
$c$ = 12.0432 (6) Å
$\alpha$ = 85.407 (2)°
$\beta$ = 85.259 (1)°
$\gamma$ = 71.256 (2)°
$V$ = 1075.74 (10) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 2.54 mm$^{-1}$
$T$ = 296 K
0.20 × 0.15 × 0.13 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.637, $T_{max}$ = 0.719
19310 measured reflections
4012 independent reflections
3441 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.059
$S$ = 1.04
4012 reflections
250 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.65 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Sn1—O1*A* | 2.23 (2) | Sn2—O3 | 2.0366 (19) |
| Sn1—O3 | 2.031 (2) | Sn2—C9 | 2.106 (5) |
| Sn1—O4 | 2.207 (3) | Sn2—C10 | 2.109 (4) |
| Sn1—C7 | 2.088 (5) | Sn2—O3$^{i}$ | 2.127 (2) |
| Sn1—C8 | 2.091 (4) | Sn2—O4$^{i}$ | 2.670 (3) |
| Sn2—O2*A* | 2.312 (17) | | |

Symmetry code: (i) $-x+1, -y, -z+1$.

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8*C*···O5$^{ii}$ | 0.96 | 2.58 | 3.103 (6) | 115 |
| C5—H5···Cg*C*$^{iii}$ | 0.93 | 2.83 | 3.513 (5) | 131 |
| C10—H10*C*···Cg*C*$^{i}$ | 0.96 | 2.80 | 3.697 (5) | 156 |

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $x, y-1, z-1$. *CgC* is the centriod of the heterocyclic ring (C13–C16/S2*A* or C13–C16/S2*B*).

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the Higher Education Commission, Islamabad, Pakistan, and Bana International, Karachi, Pakistan, for funding the purchase of the diffractometer and for technical support, respectively.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2953).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, m609-m610 [ **doi:10.1107/S1600536809015475** ]

# Octamethyldi-$\mu_3$-oxido-bis($\mu_2$-thiophene-3-acetato-$\kappa^2O$:$O'$)(thiophene-3-acetato-$\kappa O$)tetratin(IV)

**M. Danish, M. N. Tahir, N. Ahmad, A. R. Raza and M. Ibrahim**

## Comment

In continuation to our interest with the tin chemistry in various forms (Danish *et al.*, 1995, 1996), (Tahir *et al.*, 1997*a*, 1997*b*), we report here the title compound (I), (Fig. 1).

The crystal structure of bis(dicyclohexylammonium 3-thienylacetate) (Ng *et al.*, 2001) has been reported which shows disorder in the 3-thienylacetate unit. In our present complex the ligand is also in disorder. The O-atoms of chelating carboxylate are disordered over two sites with occupancy ratio of 0.65:0.35, whereas in other ligands the disorder is present at the S-atoms. In the title molecule symmetry related central four membered ring A (Sn2/O3/Sn2$^i$/O3$^i$; i = -*x* + 1, -*y*, -*z* + 1) is of course planar. The five membered rings B (C3—C5/S1/C6) and C (C13—C15/S2A/C16) are also planar. The dihedral angles between A/B, A/C and B/C are 66.28 (12)°, 77.43 (11)° and 71.23 (18)°, respectively. Due to intermolecular H-bonding, the stannoxanes are connected in pillar like polymeric form making $R_2^2(12)$ ring motifs (Bernstein *et al.*, 1995), (Fig. 2). The molecules are also stabilized due to C–H···π interactions (Table 1).

## Experimental

The complex was synthesized by refluxing $(CH_3)_2SnO$ (1.66 g, 0.01 mol) and 3-thiopheneacetic acid (1.42 g, 0.01 mol) under argon, in toluene for 4–6 h. Water formed during the reaction was continuously removed by the use of Dean-Stark apparatus. The reaction mixture was brought to room temperature and then boiled with anhydrous activated charcoal and filtered through alumina column. Toluene was removed completely from the filtrate under vacuum. The solid mass thus obtained was purified by repeated crystallization from chloroform-ethanol (8:2) mixture, to obtain colourless prisms of (I).

## Refinement

The H-atoms were positioned geometrically (C—H = 0.93–0.97Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

## Figures

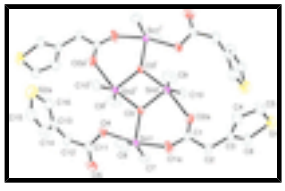


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level. H-atoms are not shown for clarity.

## Octamethyldi-μ$_3$-oxido-bis(μ$_2$-thiophene-3-acetato- κ$^2$*O*:*O*$^1$)(thiophene-3-acetato-κ*O*)tetratin(IV)

*Crystal data*

| | |
|---|---|
| $[Sn_4(CH_3)_8(C_6H_5O_2S)_4O_2]$ | $Z = 1$ |
| $M_r = 1191.79$ | $F(000) = 580$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.840$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.7330$ (5) Å | Cell parameters from 3441 reflections |
| $b = 9.7403$ (5) Å | $\theta = 2.2$–$25.5°$ |
| $c = 12.0432$ (6) Å | $\mu = 2.54$ mm$^{-1}$ |
| $\alpha = 85.407$ (2)° | $T = 296$ K |
| $\beta = 85.259$ (1)° | Prism, colourless |
| $\gamma = 71.256$ (2)° | 0.20 × 0.15 × 0.13 mm |
| $V = 1075.74$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker Kappa APEXII CCD diffractometer | 4012 independent reflections |
| Radiation source: fine-focus sealed tube | 3441 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.025$ |
| Detector resolution: 7.80 pixels mm$^{-1}$ | $\theta_{max} = 25.5°$, $\theta_{min} = 2.2°$ |
| ω scans | $h = -11 \rightarrow 11$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $k = -11 \rightarrow 11$ |
| $T_{min} = 0.637$, $T_{max} = 0.719$ | $l = -14 \rightarrow 14$ |
| 19310 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.024$ | H-atom parameters constrained |
| $wR(F^2) = 0.059$ | $w = 1/[\sigma^2(F_o^2) + (0.0219P)^2 + 1.4193P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.03$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 4012 reflections | $\Delta\rho_{max} = 0.84$ e Å$^{-3}$ |
| 250 parameters | $\Delta\rho_{min} = -0.65$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.00156 (19) |

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Sn1 | 0.18885 (2) | 0.25808 (2) | 0.45386 (2) | 0.0444 (1) | |
| Sn2 | 0.48666 (2) | −0.09190 (2) | 0.39587 (2) | 0.0446 (1) | |
| S1 | 0.27895 (18) | −0.25877 (16) | −0.05837 (11) | 0.0934 (5) | |
| S2A | 0.3409 (3) | 0.25077 (19) | 0.99888 (15) | 0.1310 (8) | 0.635 |
| O1A | 0.1177 (13) | 0.137 (3) | 0.333 (2) | 0.076 (4) | 0.65 (6) |
| O2A | 0.3179 (12) | −0.023 (3) | 0.2610 (14) | 0.065 (4) | 0.65 (6) |
| O3 | 0.3779 (2) | 0.0937 (2) | 0.47382 (18) | 0.0410 (7) | |
| O4 | 0.2813 (3) | 0.3298 (3) | 0.5913 (2) | 0.0584 (9) | |
| O5 | 0.0925 (4) | 0.5232 (4) | 0.5897 (3) | 0.1044 (16) | |
| C1 | 0.1856 (4) | 0.0434 (4) | 0.2645 (3) | 0.0497 (12) | |
| C2 | 0.0913 (4) | 0.0161 (4) | 0.1808 (3) | 0.0562 (12) | |
| C3 | 0.1613 (4) | −0.1092 (4) | 0.1087 (3) | 0.0532 (12) | |
| C4 | 0.1850 (5) | −0.2556 (5) | 0.1418 (4) | 0.0771 (19) | |
| C5 | 0.2468 (5) | −0.3522 (5) | 0.0595 (4) | 0.0719 (16) | |
| C6 | 0.2094 (6) | −0.0968 (5) | 0.0020 (4) | 0.0756 (19) | |
| C7 | 0.2415 (5) | 0.4034 (5) | 0.3342 (4) | 0.0789 (17) | |
| C8 | 0.0351 (4) | 0.1981 (5) | 0.5611 (4) | 0.0822 (18) | |
| C9 | 0.3936 (5) | −0.2493 (5) | 0.4656 (5) | 0.089 (2) | |
| C10 | 0.6134 (5) | −0.0291 (5) | 0.2633 (3) | 0.0712 (16) | |
| C11 | 0.2064 (5) | 0.4535 (4) | 0.6276 (3) | 0.0628 (14) | |
| C12 | 0.2698 (6) | 0.5070 (5) | 0.7194 (4) | 0.0832 (19) | |
| C13 | 0.2700 (5) | 0.4165 (4) | 0.8259 (3) | 0.0607 (14) | |
| C14 | 0.1451 (6) | 0.4020 (6) | 0.8834 (4) | 0.0840 (19) | |
| C15 | 0.1689 (6) | 0.3121 (5) | 0.9827 (4) | 0.0761 (19) | |
| C16 | 0.3894 (5) | 0.3378 (6) | 0.8800 (4) | 0.0839 (19) | |
| S2B | 0.3409 (3) | 0.25077 (19) | 0.99888 (15) | 0.1310 (8) | 0.365 |
| O2B | 0.283 (5) | −0.0624 (18) | 0.299 (4) | 0.065 (7) | 0.35 (6) |
| O1B | 0.156 (5) | 0.168 (2) | 0.296 (3) | 0.062 (7) | 0.35 (6) |
| H2A | 0.00668 | 0.00014 | 0.22101 | 0.0672* | |
| H4 | 0.16091 | −0.28575 | 0.21394 | 0.0921* | |
| H5 | 0.26718 | −0.45241 | 0.06791 | 0.0864* | |
| H7A | 0.19235 | 0.40649 | 0.26765 | 0.1183* | |
| H7B | 0.34458 | 0.37212 | 0.31712 | 0.1183* | |
| H6A | 0.20504 | −0.00826 | −0.03533 | 0.0906* | |

| | | | | |
|---|---|---|---|---|
| H2B | 0.05705 | 0.10329 | 0.13256 | 0.0672* |
| H8B | 0.05988 | 0.09419 | 0.56672 | 0.1230* |
| H8C | −0.05934 | 0.23970 | 0.53209 | 0.1230* |
| H9A | 0.30262 | −0.20216 | 0.50480 | 0.1329* |
| H9B | 0.45826 | −0.31449 | 0.51661 | 0.1329* |
| H9C | 0.37745 | −0.30285 | 0.40721 | 0.1329* |
| H10A | 0.67382 | 0.01893 | 0.29210 | 0.1063* |
| H10B | 0.55061 | 0.03594 | 0.21106 | 0.1063* |
| H10C | 0.67335 | −0.11358 | 0.22649 | 0.1063* |
| H12A | 0.36857 | 0.50390 | 0.69644 | 0.0997* |
| H12B | 0.21327 | 0.60710 | 0.73188 | 0.0997* |
| H14 | 0.05271 | 0.44812 | 0.85838 | 0.1013* |
| H15 | 0.09708 | 0.29176 | 1.03071 | 0.0912* |
| H16A | 0.48440 | 0.33181 | 0.85601 | 0.1007* |
| H7C | 0.21167 | 0.49849 | 0.36272 | 0.1183* |
| H8A | 0.03409 | 0.23280 | 0.63361 | 0.1230* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sn1 | 0.0437 (1) | 0.0386 (1) | 0.0463 (2) | −0.0034 (1) | −0.0056 (1) | −0.0128 (1) |
| Sn2 | 0.0470 (1) | 0.0397 (1) | 0.0452 (2) | −0.0066 (1) | −0.0063 (1) | −0.0177 (1) |
| S1 | 0.1234 (11) | 0.0908 (9) | 0.0681 (8) | −0.0294 (8) | −0.0098 (7) | −0.0323 (7) |
| S2A | 0.206 (2) | 0.0932 (11) | 0.0868 (11) | −0.0321 (12) | −0.0320 (12) | −0.0049 (9) |
| O1A | 0.058 (4) | 0.088 (8) | 0.084 (8) | −0.016 (4) | −0.007 (4) | −0.050 (7) |
| O2A | 0.054 (4) | 0.091 (10) | 0.051 (5) | −0.015 (4) | −0.010 (3) | −0.032 (5) |
| O3 | 0.0391 (11) | 0.0368 (12) | 0.0424 (12) | −0.0025 (9) | −0.0042 (9) | −0.0133 (9) |
| O4 | 0.0644 (16) | 0.0503 (14) | 0.0575 (16) | −0.0070 (12) | −0.0136 (12) | −0.0216 (12) |
| O5 | 0.099 (3) | 0.078 (2) | 0.108 (3) | 0.0243 (19) | −0.031 (2) | −0.036 (2) |
| C1 | 0.056 (2) | 0.051 (2) | 0.047 (2) | −0.0207 (18) | −0.0110 (17) | −0.0073 (17) |
| C2 | 0.063 (2) | 0.057 (2) | 0.052 (2) | −0.0193 (18) | −0.0162 (18) | −0.0092 (17) |
| C3 | 0.061 (2) | 0.057 (2) | 0.049 (2) | −0.0237 (18) | −0.0167 (17) | −0.0112 (17) |
| C4 | 0.103 (4) | 0.065 (3) | 0.073 (3) | −0.041 (3) | 0.002 (3) | −0.008 (2) |
| C5 | 0.095 (3) | 0.052 (2) | 0.077 (3) | −0.033 (2) | 0.002 (2) | −0.019 (2) |
| C6 | 0.116 (4) | 0.063 (3) | 0.052 (3) | −0.030 (3) | −0.016 (2) | −0.010 (2) |
| C7 | 0.099 (3) | 0.062 (3) | 0.059 (3) | −0.006 (2) | 0.000 (2) | 0.008 (2) |
| C8 | 0.051 (2) | 0.075 (3) | 0.117 (4) | −0.019 (2) | 0.014 (2) | −0.008 (3) |
| C9 | 0.066 (3) | 0.067 (3) | 0.143 (5) | −0.033 (2) | −0.002 (3) | −0.016 (3) |
| C10 | 0.088 (3) | 0.065 (3) | 0.047 (2) | −0.008 (2) | 0.007 (2) | −0.0032 (19) |
| C11 | 0.083 (3) | 0.049 (2) | 0.054 (2) | −0.013 (2) | −0.009 (2) | −0.0174 (18) |
| C12 | 0.137 (4) | 0.069 (3) | 0.058 (3) | −0.047 (3) | −0.012 (3) | −0.021 (2) |
| C13 | 0.077 (3) | 0.059 (2) | 0.052 (2) | −0.024 (2) | −0.005 (2) | −0.0255 (19) |
| C14 | 0.076 (3) | 0.085 (3) | 0.095 (4) | −0.028 (3) | 0.009 (3) | −0.032 (3) |
| C15 | 0.095 (4) | 0.067 (3) | 0.072 (3) | −0.037 (3) | 0.017 (3) | −0.013 (2) |
| C16 | 0.076 (3) | 0.098 (4) | 0.079 (3) | −0.022 (3) | −0.008 (2) | −0.032 (3) |
| S2B | 0.206 (2) | 0.0932 (11) | 0.0868 (11) | −0.0321 (12) | −0.0320 (12) | −0.0049 (9) |
| O2B | 0.075 (12) | 0.052 (7) | 0.076 (15) | −0.021 (5) | −0.033 (12) | −0.012 (7) |
| O1B | 0.076 (15) | 0.047 (7) | 0.062 (11) | −0.011 (6) | −0.025 (9) | −0.021 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Sn1—O1A | 2.23 (2) | C3—C6 | 1.341 (6) |
| Sn1—O3 | 2.031 (2) | C4—C5 | 1.384 (7) |
| Sn1—O4 | 2.207 (3) | C11—C12 | 1.512 (7) |
| Sn1—C7 | 2.088 (5) | C12—C13 | 1.497 (6) |
| Sn1—C8 | 2.091 (4) | C13—C16 | 1.355 (7) |
| Sn1—O1B | 2.24 (4) | C13—C14 | 1.390 (8) |
| Sn2—O2A | 2.312 (17) | C14—C15 | 1.414 (7) |
| Sn2—O3 | 2.0366 (19) | C2—H2A | 0.9700 |
| Sn2—C9 | 2.106 (5) | C2—H2B | 0.9700 |
| Sn2—C10 | 2.109 (4) | C4—H4 | 0.9300 |
| Sn2—O3$^{i}$ | 2.127 (2) | C5—H5 | 0.9300 |
| Sn2—O4$^{i}$ | 2.670 (3) | C6—H6A | 0.9300 |
| Sn2—O2B | 2.31 (5) | C7—H7A | 0.9600 |
| Sn2—Sn2$^{i}$ | 3.2694 (4) | C7—H7B | 0.9600 |
| S1—C5 | 1.686 (5) | C7—H7C | 0.9600 |
| S1—C6 | 1.701 (5) | C8—H8A | 0.9600 |
| S2A—C15 | 1.609 (7) | C8—H8B | 0.9600 |
| S2A—C16 | 1.715 (5) | C8—H8C | 0.9600 |
| S2B—C16 | 1.715 (5) | C9—H9A | 0.9600 |
| S2B—C15 | 1.609 (7) | C9—H9B | 0.9600 |
| O1A—C1 | 1.26 (3) | C9—H9C | 0.9600 |
| O1B—C1 | 1.24 (2) | C10—H10A | 0.9600 |
| O2A—C1 | 1.240 (19) | C10—H10B | 0.9600 |
| O2B—C1 | 1.23 (3) | C10—H10C | 0.9600 |
| O4—C11 | 1.281 (5) | C12—H12A | 0.9700 |
| O5—C11 | 1.204 (6) | C12—H12B | 0.9700 |
| C1—C2 | 1.511 (5) | C14—H14 | 0.9300 |
| C2—C3 | 1.498 (5) | C15—H15 | 0.9300 |
| C3—C4 | 1.399 (6) | C16—H16A | 0.9300 |
| O1A—Sn1—O3 | 91.9 (6) | C3—C4—C5 | 115.2 (4) |
| O1A—Sn1—O4 | 167.3 (7) | S1—C5—C4 | 109.0 (3) |
| O1A—Sn1—C7 | 95.5 (6) | S1—C6—C3 | 113.4 (3) |
| O1A—Sn1—C8 | 82.7 (5) | O4—C11—C12 | 116.3 (4) |
| O3—Sn1—O4 | 77.69 (9) | O4—C11—O5 | 121.5 (4) |
| O3—Sn1—C7 | 104.94 (15) | O5—C11—C12 | 122.2 (4) |
| O3—Sn1—C8 | 104.92 (14) | C11—C12—C13 | 111.4 (4) |
| O1B—Sn1—O3 | 90.8 (9) | C12—C13—C14 | 124.0 (5) |
| O4—Sn1—C7 | 94.25 (15) | C12—C13—C16 | 125.7 (5) |
| O4—Sn1—C8 | 92.93 (15) | C14—C13—C16 | 110.4 (4) |
| O1B—Sn1—O4 | 164.9 (12) | C13—C14—C15 | 115.1 (5) |
| C7—Sn1—C8 | 150.12 (18) | S2A—C15—C14 | 108.6 (4) |
| O1B—Sn1—C7 | 79.1 (9) | S2B—C15—C14 | 108.6 (4) |
| O1B—Sn1—C8 | 99.6 (11) | S2A—C16—C13 | 110.5 (4) |
| O2A—Sn2—O3 | 89.1 (6) | S2B—C16—C13 | 110.5 (4) |
| O2A—Sn2—C9 | 90.5 (6) | C1—C2—H2A | 108.00 |

| | | | |
|---|---|---|---|
| O2A—Sn2—C10 | 80.5 (4) | C1—C2—H2B | 108.00 |
| Sn2$^{i}$—Sn2—O2A | 128.1 (6) | C3—C2—H2A | 108.00 |
| O2A—Sn2—O3$^{i}$ | 164.4 (7) | C3—C2—H2B | 108.00 |
| O2A—Sn2—O4$^{i}$ | 128.2 (6) | H2A—C2—H2B | 107.00 |
| O3—Sn2—C9 | 105.78 (15) | C3—C4—H4 | 122.00 |
| O3—Sn2—C10 | 105.39 (14) | C5—C4—H4 | 122.00 |
| O2B—Sn2—O3 | 89.1 (7) | S1—C5—H5 | 126.00 |
| Sn2$^{i}$—Sn2—O3 | 39.25 (6) | C4—C5—H5 | 125.00 |
| O3—Sn2—O3$^{i}$ | 76.53 (8) | S1—C6—H6A | 123.00 |
| O3—Sn2—O4$^{i}$ | 142.67 (8) | C3—C6—H6A | 123.00 |
| C9—Sn2—C10 | 147.33 (19) | Sn1—C7—H7A | 109.00 |
| O2B—Sn2—C9 | 73.5 (9) | Sn1—C7—H7B | 110.00 |
| Sn2$^{i}$—Sn2—C9 | 105.84 (16) | Sn1—C7—H7C | 109.00 |
| O3$^{i}$—Sn2—C9 | 99.16 (16) | H7A—C7—H7B | 109.00 |
| O4$^{i}$—Sn2—C9 | 78.01 (15) | H7A—C7—H7C | 109.00 |
| O2B—Sn2—C10 | 97.5 (12) | H7B—C7—H7C | 109.00 |
| Sn2$^{i}$—Sn2—C10 | 104.38 (12) | Sn1—C8—H8A | 109.00 |
| O3$^{i}$—Sn2—C10 | 97.34 (14) | Sn1—C8—H8B | 109.00 |
| O4$^{i}$—Sn2—C10 | 83.18 (14) | Sn1—C8—H8C | 109.00 |
| Sn2$^{i}$—Sn2—O2B | 127.4 (8) | H8A—C8—H8B | 110.00 |
| O2B—Sn2—O3$^{i}$ | 161.6 (11) | H8A—C8—H8C | 109.00 |
| O2B—Sn2—O4$^{i}$ | 126.4 (5) | H8B—C8—H8C | 109.00 |
| Sn2$^{i}$—Sn2—O3$^{i}$ | 37.29 (5) | Sn2—C9—H9A | 109.00 |
| Sn2$^{i}$—Sn2—O4$^{i}$ | 103.52 (6) | Sn2—C9—H9B | 109.00 |
| O3$^{i}$—Sn2—O4$^{i}$ | 66.28 (8) | Sn2—C9—H9C | 109.00 |
| C5—S1—C6 | 92.5 (2) | H9A—C9—H9B | 109.00 |
| C15—S2A—C16 | 95.4 (3) | H9A—C9—H9C | 109.00 |
| C15—S2B—C16 | 95.4 (3) | H9B—C9—H9C | 110.00 |
| Sn1—O1A—C1 | 133.2 (11) | Sn2—C10—H10A | 109.00 |
| Sn1—O1B—C1 | 134 (2) | Sn2—C10—H10B | 109.00 |
| Sn2—O2A—C1 | 132.8 (12) | Sn2—C10—H10C | 109.00 |
| Sn2—O2B—C1 | 134 (2) | H10A—C10—H10B | 109.00 |
| Sn2—O3—Sn2$^{i}$ | 103.47 (9) | H10A—C10—H10C | 110.00 |
| Sn1—O3—Sn2$^{i}$ | 120.70 (10) | H10B—C10—H10C | 110.00 |
| Sn1—O3—Sn2 | 135.83 (11) | C11—C12—H12A | 109.00 |
| Sn2$^{i}$—O4—C11 | 149.5 (3) | C11—C12—H12B | 109.00 |
| Sn1—O4—Sn2$^{i}$ | 95.14 (9) | C13—C12—H12A | 109.00 |
| Sn1—O4—C11 | 115.4 (3) | C13—C12—H12B | 109.00 |
| O1A—C1—O2A | 125.9 (13) | H12A—C12—H12B | 108.00 |
| O1A—C1—C2 | 114.1 (9) | C13—C14—H14 | 122.00 |
| O2A—C1—C2 | 120.0 (10) | C15—C14—H14 | 122.00 |
| O1B—C1—O2B | 125 (3) | S2A—C15—H15 | 126.00 |
| O1B—C1—C2 | 118 (2) | C14—C15—H15 | 126.00 |
| O2B—C1—C2 | 116.6 (18) | S2B—C15—H15 | 126.00 |

| | | | |
|---|---|---|---|
| C1—C2—C3 | 116.3 (3) | S2A—C16—H16A | 125.00 |
| C2—C3—C4 | 125.4 (4) | C13—C16—H16A | 125.00 |
| C2—C3—C6 | 124.6 (4) | S2B—C16—H16A | 125.00 |
| C4—C3—C6 | 110.0 (4) | | |
| O3—Sn1—O1A—C1 | −29 (2) | C10—Sn2—Sn2$^{i}$—O2A$^{i}$ | −90.9 (6) |
| C7—Sn1—O1A—C1 | 76 (2) | C10—Sn2—Sn2$^{i}$—O3$^{i}$ | −83.16 (16) |
| C8—Sn1—O1A—C1 | −134 (2) | C10—Sn2—Sn2$^{i}$—C9$^{i}$ | 12.55 (19) |
| O1A—Sn1—O3—Sn2 | 11.1 (6) | C10—Sn2—Sn2$^{i}$—C10$^{i}$ | 180.0 (2) |
| O1A—Sn1—O3—Sn2$^{i}$ | −168.5 (6) | O3$^{i}$—Sn2—Sn2$^{i}$—O3 | 180.00 (14) |
| O4—Sn1—O3—Sn2 | −176.29 (17) | O3$^{i}$—Sn2—Sn2$^{i}$—O4 | 176.85 (11) |
| O4—Sn1—O3—Sn2$^{i}$ | 4.13 (11) | O4$^{i}$—Sn2—Sn2$^{i}$—O3 | −176.85 (11) |
| C7—Sn1—O3—Sn2 | −85.1 (2) | O4$^{i}$—Sn2—Sn2$^{i}$—O4 | 180.00 (8) |
| C7—Sn1—O3—Sn2$^{i}$ | 95.29 (17) | O3—Sn2—O3$^{i}$—Sn1$^{i}$ | −179.70 (13) |
| C8—Sn1—O3—Sn2 | 94.0 (2) | O3—Sn2—O3$^{i}$—Sn2$^{i}$ | 0.00 (10) |
| C8—Sn1—O3—Sn2$^{i}$ | −85.63 (17) | C9—Sn2—O3$^{i}$—Sn1$^{i}$ | 76.14 (17) |
| O3—Sn1—O4—C11 | 178.3 (3) | C9—Sn2—O3$^{i}$—Sn2$^{i}$ | −104.16 (16) |
| O3—Sn1—O4—Sn2$^{i}$ | −2.84 (8) | C10—Sn2—O3$^{i}$—Sn1$^{i}$ | −75.56 (16) |
| C7—Sn1—O4—C11 | 73.9 (3) | C10—Sn2—O3$^{i}$—Sn2$^{i}$ | 104.14 (15) |
| C7—Sn1—O4—Sn2$^{i}$ | −107.23 (15) | O2A—Sn2—O4$^{i}$—Sn1$^{i}$ | 170.4 (6) |
| C8—Sn1—O4—C11 | −77.1 (3) | O2A—Sn2—O4$^{i}$—C11$^{i}$ | −7.7 (8) |
| C8—Sn1—O4—Sn2$^{i}$ | 101.80 (14) | O3—Sn2—O4$^{i}$—Sn1$^{i}$ | −8.27 (18) |
| O3—Sn2—O2A—C1 | −35 (2) | O3—Sn2—O4$^{i}$—C11$^{i}$ | 173.7 (5) |
| C9—Sn2—O2A—C1 | 71 (2) | C9—Sn2—O4$^{i}$—Sn1$^{i}$ | −108.63 (18) |
| C10—Sn2—O2A—C1 | −140 (2) | C9—Sn2—O4$^{i}$—C11$^{i}$ | 73.3 (5) |
| Sn2$^{i}$—Sn2—O2A—C1 | −39 (2) | C10—Sn2—O4$^{i}$—Sn1$^{i}$ | 98.23 (15) |
| O4$^{i}$—Sn2—O2A—C1 | 146.3 (19) | C10—Sn2—O4$^{i}$—C11$^{i}$ | −79.9 (5) |
| O2A—Sn2—O3—Sn1 | 6.5 (5) | C6—S1—C5—C4 | −0.7 (4) |
| O2A—Sn2—O3—Sn2$^{i}$ | −173.9 (5) | C5—S1—C6—C3 | −0.3 (5) |
| C9—Sn2—O3—Sn1 | −83.8 (2) | C16—S2A—C15—C14 | 0.2 (4) |
| C9—Sn2—O3—Sn2$^{i}$ | 95.88 (17) | C15—S2A—C16—C13 | 0.0 (4) |
| C10—Sn2—O3—Sn1 | 86.34 (19) | Sn1—O1A—C1—O2A | 13 (3) |
| C10—Sn2—O3—Sn2$^{i}$ | −94.03 (15) | Sn1—O1A—C1—C2 | −166.7 (15) |
| Sn2$^{i}$—Sn2—O3—Sn1 | −179.6 (2) | Sn2—O2A—C1—O1A | 29 (3) |
| O3$^{i}$—Sn2—O3—Sn1 | −179.63 (17) | Sn2—O2A—C1—C2 | −152.2 (14) |
| O3$^{i}$—Sn2—O3—Sn2$^{i}$ | 0.00 (8) | Sn1—O4—C11—O5 | 1.2 (5) |
| O4$^{i}$—Sn2—O3—Sn1 | −174.57 (12) | Sn1—O4—C11—C12 | −178.2 (3) |
| O4$^{i}$—Sn2—O3—Sn2$^{i}$ | 5.06 (18) | Sn2$^{i}$—O4—C11—O5 | −176.6 (3) |
| O2A—Sn2—Sn2$^{i}$—O3 | 7.8 (6) | Sn2$^{i}$—O4—C11—C12 | 4.0 (7) |
| O2A—Sn2—Sn2$^{i}$—O4 | 4.6 (6) | O1A—C1—C2—C3 | −171.2 (13) |
| O2A—Sn2—Sn2$^{i}$—O2A$^{i}$ | −180.0 (8) | O2A—C1—C2—C3 | 9.5 (13) |
| O2A—Sn2—Sn2$^{i}$—O3$^{i}$ | −172.2 (6) | C1—C2—C3—C4 | 78.1 (5) |
| O2A—Sn2—Sn2$^{i}$—C9$^{i}$ | −76.5 (6) | C1—C2—C3—C6 | −102.5 (5) |

| | | | |
|---|---|---|---|
| O2A—Sn2—Sn2$^{i}$—C10$^{i}$ | 90.9 (6) | C2—C3—C4—C5 | 177.7 (4) |
| O3—Sn2—Sn2$^{i}$—O4 | −3.15 (11) | C6—C3—C4—C5 | −1.7 (6) |
| O3—Sn2—Sn2$^{i}$—O2A$^{i}$ | 172.2 (6) | C2—C3—C6—S1 | −178.3 (3) |
| O3—Sn2—Sn2$^{i}$—O3$^{i}$ | −180.00 (14) | C4—C3—C6—S1 | 1.2 (6) |
| O3—Sn2—Sn2$^{i}$—C9$^{i}$ | −84.29 (17) | C3—C4—C5—S1 | 1.5 (6) |
| O3—Sn2—Sn2$^{i}$—C10$^{i}$ | 83.16 (16) | O4—C11—C12—C13 | −68.4 (5) |
| C9—Sn2—Sn2$^{i}$—O3 | −95.71 (17) | O5—C11—C12—C13 | 112.2 (5) |
| C9—Sn2—Sn2$^{i}$—O4 | −98.86 (15) | C11—C12—C13—C14 | −61.4 (6) |
| C9—Sn2—Sn2$^{i}$—O2A$^{i}$ | 76.5 (6) | C11—C12—C13—C16 | 118.7 (5) |
| C9—Sn2—Sn2$^{i}$—O3$^{i}$ | 84.29 (17) | C12—C13—C14—C15 | −179.6 (4) |
| C9—Sn2—Sn2$^{i}$—C9$^{i}$ | −180.0 (2) | C16—C13—C14—C15 | 0.3 (6) |
| C9—Sn2—Sn2$^{i}$—C10$^{i}$ | −12.55 (19) | C12—C13—C16—S2A | 179.8 (4) |
| C10—Sn2—Sn2$^{i}$—O3 | 96.85 (16) | C14—C13—C16—S2A | −0.2 (5) |
| C10—Sn2—Sn2$^{i}$—O4 | 93.70 (15) | C13—C14—C15—S2A | −0.4 (6) |

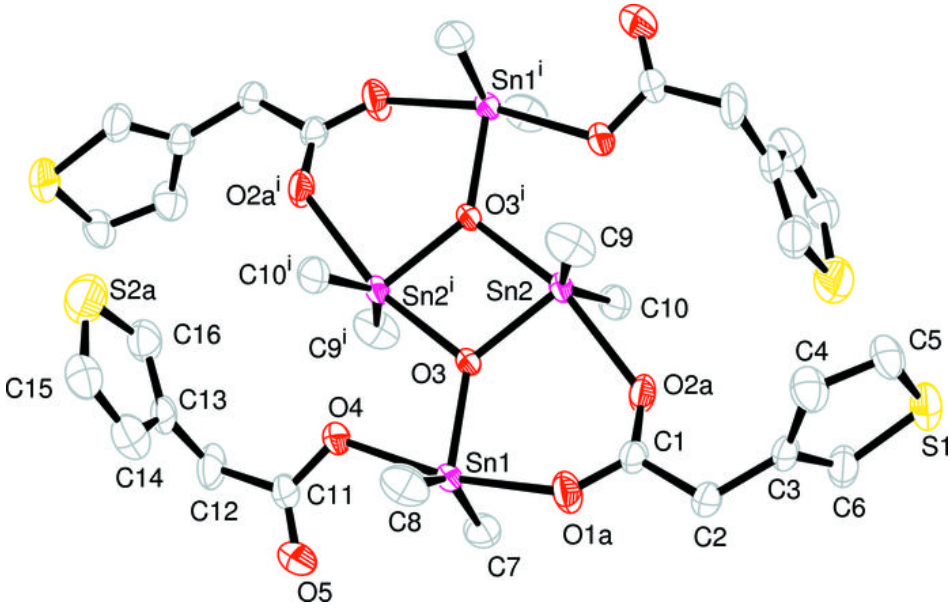
Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8C···O5$^{ii}$ | 0.96 | 2.58 | 3.103 (6) | 115 |
| C5—H5···CgC$^{iii}$ | 0.93 | 2.83 | 3.513 (5) | 131 |
| C10—H10C···CgC$^{i}$ | 0.96 | 2.80 | 3.697 (5) | 156 |

Symmetry codes: (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*−1; (i) −*x*+1, −*y*, −*z*+1.

**Fig. 1**


Sn1i
O2ai
O3i
C9
C10i
Sn2i
Sn2
C10
S2a
C16
C9i
O3
C4
C5
C15
C13
O4
O2a
S1
C1
Sn1
C14
C12
C11
C8
O1a
C3
C6
C2
C7
O5