metal-organic compounds

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Diacetatodi-tert-butyltin(IV)

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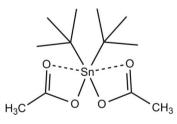
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Key indicators: single-crystal X-ray study; T = 100 K; mean σ (C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.046; data-to-parameter ratio = 21.5.

The title compound, $[Sn(C_4H_9)_2(CH_3COO)_2]$, was synthesized in order to study the influence of large organic groups on the molecular structure of diorganotin diacetates. The title compound exhibits the same structure type as other diorganotin(IV) diacetates characterized by an unsymmetrical bidentate bonding mode of the two acetate groups to tin. The influence of the *t*-butyl groups on this molecular structure is expressed in two significant differences: tin—carbon bond lengths are much more longer than in the other diacetates, as are the additional interactions of the acetate groups with the tin atom. Intermolecular interactions are restricted to C— $H \cdots O$ ones similar to those in the other diacetates, giving rise to a chain-like arrangement of the molecules with the tin atoms and acetate groups in the propagation plane.

Related literature

For background to diorganotin(IV) carboxylates, see: Tiekink (1991) and to diorganotin(IV) diacetates, see: Alcock *et al.* (1992); Lockhart *et al.* (1987); Mistry *et al.* (1995).



Experimental

Crystal data [Sn(C₄H₉)₂(C₂H₃O₂)₂] $M_r = 351.00$ Monoclinic, $P2_1/n$ a = 6.1039 (3) Å b = 15.3928 (7) Å c = 15.9601 (8) Å $\beta = 95.462$ (2)°

 $V = 1492.74 (12) Å^{3}$ Z = 4Mo K\alpha radiation $\mu = 1.71 \text{ mm}^{-1}$ T = 100 K $0.14 \times 0.06 \times 0.04 \text{ mm}$

Data collection

Bruker APEXII CCD

diffractometer Absorption correction: multi-scan (*SADABS*; Bruker, 2009) $T_{\min} = 0.791, T_{\max} = 0.939$

Refinement

| $R[F^2 > 2\sigma(F^2)] = 0.023$ | 167 parameters |
|---------------------------------|--|
| $wR(F^2) = 0.046$ | H-atom parameters constrained |
| S = 1.04 | $\Delta \rho_{\rm max} = 0.59 \text{ e } \text{\AA}^{-3}$ |
| 3590 reflections | $\Delta \rho_{\rm min} = -0.51 \text{ e } \text{\AA}^{-3}$ |

76636 measured reflections

 $R_{\rm int} = 0.081$

3590 independent reflections

2980 reflections with $I > 2\sigma(I)$

Table 1

Selected bond lengths (Å).

| Sn1-O21 | 2.1001 (14) | O11-C15 | 1.304 (3) |
|---------|-------------|---------|-----------|
| Sn1-O11 | 2.1002 (14) | O12-C15 | 1.235 (3) |
| Sn1-C11 | 2.175 (2) | O21-C25 | 1.304 (3) |
| Sn1-C21 | 2.176 (2) | O22-C25 | 1.239 (3) |

| Tabl | e 2 | |
|------|-----|--|
|------|-----|--|

| The days and have d | | (Å | 0) |
|---------------------|----------|-----|----|
| Hydrogen-bond | geometry | А, |). |

| $D - H \cdot \cdot \cdot A$ | $D-\mathrm{H}$ | $H \cdots A$ | $D \cdots A$ | $D - \mathbf{H} \cdot \cdot \cdot A$ |
|---------------------------------------|----------------|--------------|--------------|--------------------------------------|
| $C12-H12C\cdots O21^{i}$ | 0.98 | 2.54 | 3.362 (3) | 142 |
| $C22-H22C\cdots O11^{i}$ | 0.98 | 2.65 | 3.584 (3) | 160 |
| $C16-H16C \cdot \cdot \cdot O22^{ii}$ | 0.98 | 2.69 | 3.636 (3) | 163 |
| $C16-H16A\cdots O22^{iii}$ | 0.98 | 2.60 | 3.518 (3) | 155 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

We thank the Deutsche Forschungsgemeinschaft and the Government of Lower Saxony for their financial support in the acquisition of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2086).

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supporting information

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Diacetatodi-tert-butyltin(IV)

Martin Reichelt and Hans Reuter

S1. Comment

Diorganotin(IV) dicarboxylates, R_2 Sn(O₂CR')₂, belong to the class of diorganotin compounds, R_2 Sn X_2 , with univalent anions *X*, such as the halides (*X* = F, Cl, Br, I) or alkoxides (*X* = OR'). In contrast to these anions, that behave as unidentate substitutents, the carboxylate groups, O₂CR', can act *via* its two oxygen atoms as a bidentate ligand in a more or less symmetrical or unsymmetrical coordination mode giving rise to additional intra- or intermolecular interactions (Tiekink, 1991). In the case of diacetates, R' = Me, this was formerly shown for R = phenyl (Alcock *et al.* 1992) and R =methyl (Lockhart *et al.* 1987, α -modification; Mistry *et al.* 1995, β -modification) both revealing in solid state the same molecular structure type with a strongly unsymmetrical bonding mode of the acetate groups. On this background it was interesting to see whether the larger *t*-butyl groups are compatible with that structure type or not.

The asymmetric unit of the title compound (Fig. 1) consists of one formula unit with all atoms in general positions although the molecule displays a pseudo twofold rotation axis [midway C11/C21 - Sn - midway O11/O21]. In a first approximation, the tin atom is fourfold coordinated by the two *t*-butyl groups and an oxygen atom of each acetate group. Both Sn—C bond lengths are almost equal as are both Sn—O bond lengths, too (see Table 1). The last ones are comparable with Sn—O bond lengths in the other diacetates [$d(\text{Sn}_O) = 2.076$ (4), 2.079 (4), R = Ph; 2 x 2.106 (2), $R = \alpha$ -Me, 2.098 (2), 2.094 (2), $R = \beta$ -Me]. In comparison to the methyl compounds with Sn—C bond lengths of 2 x 2.098 (3) Å [α], respectively 2.096 (3), 2.088 (3) Å [β] and the phenyl compound [2.119 (5), 2.110 (6) Å] Sn—C bonds of the *tert*-butyl groups are considerable longer. From the bond angles of 138.97 (7)° between the *t*-butyl groups and 79.93 (6)° between the two oxygen atoms, the coordination polyhedron is compressed to a tetragonal disphenoid (Fig. 2). Obviously, this distortion is typical for diacetates [C—Sn—C = 131.4°, R = Ph; 135.9 (2)°(1)°, $R = \alpha$ -Me; 133.8 (2)°, $R = \beta$ -Me; O—Sn—O = 82.0 (3)°, R = Ph; 79.5 (1)°, $R = \alpha$ -Me; 80.1 (1)°, $R = \beta$ -Me].

The coordination sphere of the tin atom is completed by the other two oxygen atoms of the acetate groups that undergo a much more weaker interaction with the tin atom $[d(\text{Sn} \cdots \text{O}) = 2.689 (1) \text{ Å to } \text{O22}, 2.647 (2) \text{ Å to } \text{O12}]$, resulting in a very unsymmetrical bidentate coordination mode of the acetate groups (Fig. 2). This is also reflected in two different C— O distances for each acetate group (Table 1). Again, within the molecular structures of the other diacetates a similar coordination behaviour is observed but Sn···O interactions are considerably stronger [2.583 (4), 2.527 (5) Å, R = Ph; 2 x 2.539 (2) Å, $R = \alpha$ -Me; 2.563 (2), 2.595 (2) Å, $R = \beta$ -Me].

Both *t*-butyl groups are well ordered with a mean value for the C—C bonds of 1.527 (3) Å [range: 1.522 (3) - 1.530 (3) Å] and a mean C—C—C bond angle of 110.2 (4)° [range: 109.65 (3)° - 110.65 (3)°]. With respect to Sn—C—C bond angles, both *t*-butyl groups show similar effects: two angles are around the ideal tetrahedral value of 109.5°, whereas the third one is significantly smaller [107.09 (3)° for C12; 106.07 (2)° for C22].

In the solid, molecules are arranged in chains with the tin atoms and acetate groups defining the propagation plane (Fig. 3). This arrangement is also characteristic for both modifications of the methyl compounds but not for the phenyl one. In the present case, the intermolecular O···Sn distances of 4.692 (1) Å [O21···Sn1¹] and 4.694 (1) Å [O11···Sn1¹], however,

are so long that seems impossible that these interactions are responsible for the supra-molecular architecture. There are, however, O…HC interactions between the acetate groups and *t*-butyl groups of neighbouring molecules (Fig. 4) that are much more attractive (Table 2). Similar interactions are found in all other diorganotin(IV) diacetates and even in the phenyl compound.

S2. Experimental

Synthesis:

0.51 g (0.68 mmol) di-*t*-butyltin oxide are dissolved in 0.25 g (4.16 mmol) of acetic acid (Fluka). The solution is stirred for 6 h at ambient temperature before the solvent is allowed to evaporate slowly. After about 1 week colourless block-like crystals are grown.

Spectroscopic studies:

Elemental analysis calcd (%) for C₅H₄O₃: C, 41.06; H, 6.89. Found: C, 40.99; H, 6.53. ¹H-NMR (CDCl₃, p.p.m.): 2.09 (s,OAc, 3H), 1.35 (s, tBu, 9H, ${}^{3}J({}^{1}H^{-119/117}Sn = 119.1/114.1 Hz)$. { ${}^{1}H$ }- ${}^{13}C$ -NMR (CDCl₃, p.p.m.): 180.59 (O₂CCH₃), 45.29 (C_a-tBu, ${}^{1}J({}^{13}C^{-119/117}Sn) = 515.3/492.4 Hz)$, 29.67 (C_b-tBu), 20.37 (O₂CCH₃). IR (ATR, cm⁻¹): 2853.6, 1601.0, 1438.3, 1367.9, 1323.9, 1160.4, 1053.5, 1018.2, 942.5, 807.9, 688.4, 620.1, 499.2.

Crystallographic studies:

A suitable single-crystal was selected under a polarization microscope and mounted on a 50 µm MicroMesh MiTeGen Micromount[™] using FROMBLIN Y perfluoropolyether (LVAC 16/6, Aldrich).

S3. Refinement

Hydrogen atoms were clearly identified in difference Fourier syntheses. Their positions were idealized and refined at calculated positions riding on the carbon atoms with C-H = 0.98 Å.

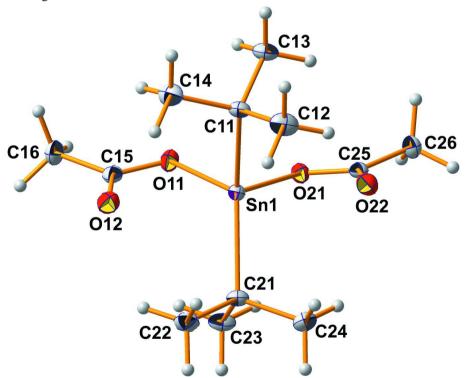


Figure 1

Molecular structure of the title compound, with 50% probability level displacement ellipsoids for non-H atoms.

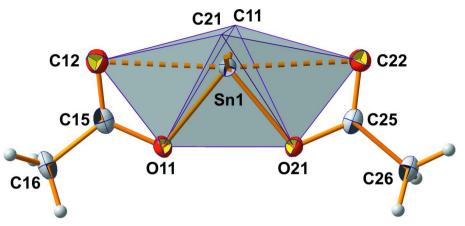


Figure 2

Polyhedron model of the coordination sphere of the tin atom; *t*-butyl groups have been omitted for clarity, weak Sn… O interactions are indicated by dashed sticks. Displacement ellipsoids for non-H atoms are shown with 50% probability level

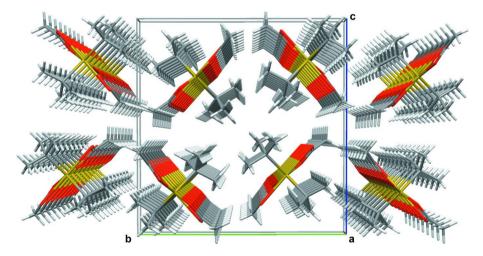


Figure 3

Perspective view of the crystal structure parallel to the crystallographic *a* axis, showing the chain-like arrangement of acetate groups and tin atoms.

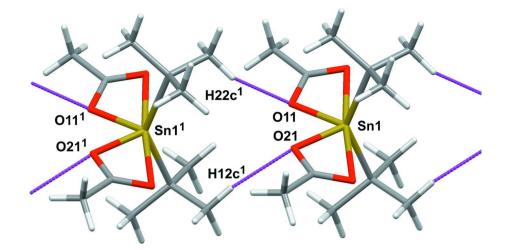


Figure 4

Intermolecular oxygen hydrogen interactions within the chain-like arrangement of the *diacetate* molecules [Symmetry operator: (1) 1 + x, y, z].

Diacetatodi-tert-butyltin(IV)

Crystal data

 $[Sn(C_4H_9)_2(C_2H_3O_2)_2]$ $M_r = 351.00$ Monoclinic, $P2_1/n$ Hall symbol: -P 2yn a = 6.1039 (3) Å b = 15.3928 (7) Å c = 15.9601 (8) Å $\beta = 95.462$ (2)° V = 1492.74 (12) Å³ Z = 4

Data collection

Bruker APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator φ and ω scans Absorption correction: multi-scan (*SADABS*; Bruker, 2009) $T_{\min} = 0.791, T_{\max} = 0.939$

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.023$ $wR(F^2) = 0.046$ S = 1.043590 reflections 167 parameters 0 restraints Primary atom site location: structure-invariant direct methods F(000) = 712 $D_x = 1.562 \text{ Mg m}^{-3}$ Mo Ka radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 6480 reflections $\theta = 2.6-25.7^{\circ}$ $\mu = 1.71 \text{ mm}^{-1}$ T = 100 KBlock, colourless $0.14 \times 0.06 \times 0.04 \text{ mm}$

76636 measured reflections 3590 independent reflections 2980 reflections with $I > 2\sigma(I)$ $R_{int} = 0.081$ $\theta_{max} = 28.0^\circ, \ \theta_{min} = 1.8^\circ$ $h = -8 \rightarrow 8$ $k = -20 \rightarrow 19$ $l = -21 \rightarrow 21$

Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0133P)^2 + 1.0511P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.002$ $\Delta\rho_{max} = 0.59$ e Å⁻³ $\Delta\rho_{min} = -0.51$ e Å⁻³

Extinction correction: *SHELXL*, Fc^{*}=kFc[1+0.001xFc² λ^3 /sin(2 θ)]^{-1/4}

Extinction coefficient: 0.00201 (16)

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 $(Å^2)$

| | x | у | Ζ | $U_{ m iso}$ */ $U_{ m eq}$ |
|------|-------------|--------------|--------------|-----------------------------|
| Sn1 | 0.19140 (2) | 0.295768 (9) | 0.285075 (8) | 0.01333 (6) |
| C11 | 0.0432 (3) | 0.20445 (14) | 0.19231 (13) | 0.0162 (4) |
| C12 | -0.1709 (3) | 0.24192 (16) | 0.14968 (14) | 0.0257 (5) |
| H12A | -0.2374 | 0.2001 | 0.1085 | 0.031 (2)* |
| H12B | -0.1396 | 0.2962 | 0.1211 | 0.031 (2)* |
| H12C | -0.2730 | 0.2534 | 0.1922 | 0.031 (2)* |
| C13 | 0.2095 (4) | 0.18975 (15) | 0.12781 (13) | 0.0216 (5) |
| H13A | 0.3485 | 0.1689 | 0.1566 | 0.031 (2)* |
| H13B | 0.2350 | 0.2445 | 0.0990 | 0.031 (2)* |
| H13C | 0.1515 | 0.1464 | 0.0865 | 0.031 (2)* |
| C14 | -0.0036 (4) | 0.11881 (15) | 0.23553 (14) | 0.0259 (5) |
| H14A | -0.1128 | 0.1285 | 0.2758 | 0.031 (2)* |
| H14B | 0.1327 | 0.0966 | 0.2654 | 0.031 (2)* |
| H14C | -0.0609 | 0.0764 | 0.1932 | 0.031 (2)* |
| C21 | 0.0894 (3) | 0.38924 (14) | 0.37595 (12) | 0.0161 (4) |
| C22 | -0.0723 (4) | 0.34722 (15) | 0.43092 (14) | 0.0245 (5) |
| H22A | -0.1180 | 0.3900 | 0.4713 | 0.030 (2)* |
| H22B | -0.0011 | 0.2980 | 0.4614 | 0.030 (2)* |
| H22C | -0.2016 | 0.3267 | 0.3953 | 0.030 (2)* |
| C23 | 0.2995 (4) | 0.41692 (15) | 0.42919 (14) | 0.0243 (5) |
| H23A | 0.2626 | 0.4591 | 0.4717 | 0.030 (2)* |
| H23B | 0.4014 | 0.4435 | 0.3928 | 0.030 (2)* |
| H23C | 0.3689 | 0.3659 | 0.4572 | 0.030 (2)* |
| C24 | -0.0185 (4) | 0.46712 (15) | 0.33009 (14) | 0.0249 (5) |
| H24A | -0.1502 | 0.4481 | 0.2950 | 0.030 (2)* |
| H24B | 0.0852 | 0.4936 | 0.2944 | 0.030 (2)* |
| H24C | -0.0601 | 0.5098 | 0.3713 | 0.030 (2)* |
| 011 | 0.4677 (2) | 0.22581 (9) | 0.33641 (9) | 0.0198 (3) |
| 012 | 0.1995 (3) | 0.18113 (10) | 0.40892 (10) | 0.0251 (4) |
| C15 | 0.3940 (4) | 0.17649 (14) | 0.39399 (13) | 0.0203 (5) |
| C16 | 0.5546 (4) | 0.11407 (16) | 0.43777 (14) | 0.0265 (5) |
| H16A | 0.5282 | 0.1099 | 0.4973 | 0.037 (4)* |
| H16B | 0.7049 | 0.1347 | 0.4333 | 0.037 (4)* |
| - | | | | |

supporting information

| H16C | 0.5357 | 0.0567 | 0.4114 | 0.037 (4)* |
|------|------------|--------------|--------------|------------|
| O21 | 0.4416 (2) | 0.36282 (9) | 0.23048 (9) | 0.0178 (3) |
| O22 | 0.1404 (2) | 0.41038 (10) | 0.15759 (9) | 0.0231 (3) |
| C25 | 0.3440 (4) | 0.40733 (13) | 0.16819 (13) | 0.0185 (5) |
| C26 | 0.4899 (4) | 0.45081 (15) | 0.11080 (14) | 0.0240 (5) |
| H26A | 0.5160 | 0.4114 | 0.0646 | 0.038 (4)* |
| H26B | 0.6306 | 0.4656 | 0.1423 | 0.038 (4)* |
| H26C | 0.4188 | 0.5039 | 0.0879 | 0.038 (4)* |
| | | | | |

| Atomic displacement parameters (| (A^2) |
|----------------------------------|---------|
|----------------------------------|---------|

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Sn1 | 0.01484 (8) | 0.01307 (8) | 0.01231 (8) | 0.00027 (6) | 0.00240 (5) | -0.00084 (6) |
| C11 | 0.0158 (10) | 0.0177 (11) | 0.0156 (10) | -0.0010 (8) | 0.0038 (8) | -0.0048 (8) |
| C12 | 0.0162 (11) | 0.0342 (14) | 0.0260 (12) | 0.0018 (10) | -0.0017 (9) | -0.0072 (10) |
| C13 | 0.0222 (11) | 0.0235 (13) | 0.0194 (11) | -0.0006 (9) | 0.0037 (9) | -0.0078 (9) |
| C14 | 0.0294 (13) | 0.0220 (12) | 0.0276 (12) | -0.0095 (10) | 0.0089 (10) | -0.0041 (10) |
| C21 | 0.0153 (10) | 0.0166 (11) | 0.0167 (10) | 0.0006 (8) | 0.0028 (8) | -0.0051 (8) |
| C22 | 0.0249 (12) | 0.0239 (13) | 0.0265 (12) | 0.0005 (10) | 0.0128 (10) | -0.0036 (10) |
| C23 | 0.0246 (12) | 0.0266 (13) | 0.0216 (12) | -0.0006 (10) | 0.0018 (9) | -0.0093 (9) |
| C24 | 0.0303 (13) | 0.0204 (12) | 0.0246 (12) | 0.0065 (10) | 0.0057 (10) | -0.0020 (9) |
| O11 | 0.0211 (8) | 0.0180 (8) | 0.0199 (8) | 0.0020 (6) | -0.0005 (6) | 0.0035 (6) |
| O12 | 0.0273 (9) | 0.0222 (9) | 0.0263 (9) | 0.0039 (7) | 0.0055 (7) | 0.0017 (7) |
| C15 | 0.0286 (13) | 0.0147 (11) | 0.0166 (11) | 0.0014 (9) | -0.0025 (9) | -0.0031 (8) |
| C16 | 0.0337 (13) | 0.0229 (12) | 0.0221 (12) | 0.0072 (10) | -0.0024 (10) | 0.0049 (10) |
| O21 | 0.0192 (8) | 0.0172 (8) | 0.0174 (7) | -0.0003 (6) | 0.0046 (6) | 0.0027 (6) |
| O22 | 0.0226 (9) | 0.0267 (9) | 0.0202 (8) | 0.0019 (7) | 0.0028 (6) | 0.0013 (6) |
| C25 | 0.0279 (12) | 0.0137 (11) | 0.0147 (10) | -0.0021 (9) | 0.0055 (9) | -0.0036 (8) |
| C26 | 0.0304 (13) | 0.0215 (13) | 0.0209 (12) | -0.0012 (10) | 0.0076 (10) | 0.0030 (9) |

Geometric parameters (Å, °)

| Sn1—O21 | 2.1001 (14) | C22—H22B | 0.9800 |
|----------|-------------|----------|-----------|
| Sn1—O11 | 2.1002 (14) | C22—H22C | 0.9800 |
| Sn1—C11 | 2.175 (2) | C23—H23A | 0.9800 |
| Sn1—C21 | 2.176 (2) | С23—Н23В | 0.9800 |
| C11—C14 | 1.527 (3) | C23—H23C | 0.9800 |
| C11—C12 | 1.528 (3) | C24—H24A | 0.9800 |
| C11—C13 | 1.530 (3) | C24—H24B | 0.9800 |
| C12—H12A | 0.9800 | C24—H24C | 0.9800 |
| C12—H12B | 0.9800 | O11—C15 | 1.304 (3) |
| C12—H12C | 0.9800 | O12—C15 | 1.235 (3) |
| C13—H13A | 0.9800 | C15—C16 | 1.497 (3) |
| С13—Н13В | 0.9800 | C16—H16A | 0.9800 |
| C13—H13C | 0.9800 | C16—H16B | 0.9800 |
| C14—H14A | 0.9800 | C16—H16C | 0.9800 |
| C14—H14B | 0.9800 | O21—C25 | 1.304 (3) |
| C14—H14C | 0.9800 | O22—C25 | 1.239 (3) |
| | | | |

| C21—C24 | 1.522 (3) | C25—C26 | 1.495 (3) |
|---------------|-------------|---------------|-------------|
| C21—C22 | 1.525 (3) | C26—H26A | 0.9800 |
| C21—C23 | 1.530 (3) | C26—H26B | 0.9800 |
| C22—H22A | 0.9800 | C26—H26C | 0.9800 |
| | 0.9000 | 020 11200 | 0.9000 |
| O21—Sn1—O11 | 79.93 (6) | C21—C22—H22B | 109.5 |
| O21—Sn1—C11 | 107.88 (7) | H22A—C22—H22B | 109.5 |
| O11—Sn1—C11 | 101.58 (7) | C21—C22—H22C | 109.5 |
| O21—Sn1—C21 | 102.54 (7) | H22A—C22—H22C | 109.5 |
| O11—Sn1—C21 | 110.43 (7) | H22B—C22—H22C | 109.5 |
| C11—Sn1—C21 | 138.97 (7) | C21—C23—H23A | 109.5 |
| C14—C11—C12 | 109.77 (18) | C21—C23—H23B | 109.5 |
| C14—C11—C13 | 109.93 (18) | H23A—C23—H23B | 109.5 |
| C12—C11—C13 | 110.51 (17) | C21—C23—H23C | 109.5 |
| C14—C11—Sn1 | 109.51 (14) | H23A—C23—H23C | 109.5 |
| C12-C11-Sn1 | 109.99 (14) | H23B—C23—H23C | 109.5 |
| C13—C11—Sn1 | 107.09 (13) | C21—C24—H24A | 109.5 |
| C11—C12—H12A | 109.5 | C21—C24—H24B | 109.5 |
| C11—C12—H12B | 109.5 | H24A—C24—H24B | 109.5 |
| H12A—C12—H12B | 109.5 | C21—C24—H24C | 109.5 |
| C11—C12—H12C | 109.5 | H24A—C24—H24C | 109.5 |
| H12A—C12—H12C | 109.5 | H24B—C24—H24C | 109.5 |
| H12B—C12—H12C | 109.5 | C15—O11—Sn1 | 104.81 (13) |
| C11—C13—H13A | 109.5 | O12—C15—O11 | 120.3 (2) |
| C11—C13—H13B | 109.5 | O12-C15-C16 | 123.1 (2) |
| H13A—C13—H13B | 109.5 | O11-C15-C16 | 116.6 (2) |
| C11—C13—H13C | 109.5 | C15-C16-H16A | 109.5 |
| H13A—C13—H13C | 109.5 | C15-C16-H16B | 109.5 |
| H13B—C13—H13C | 109.5 | H16A—C16—H16B | 109.5 |
| C11—C14—H14A | 109.5 | C15—C16—H16C | 109.5 |
| C11—C14—H14B | 109.5 | H16A—C16—H16C | 109.5 |
| H14A—C14—H14B | 109.5 | H16B—C16—H16C | 109.5 |
| C11—C14—H14C | 109.5 | C25—O21—Sn1 | 106.07 (13) |
| H14A—C14—H14C | 109.5 | O22—C25—O21 | 120.25 (19) |
| H14B—C14—H14C | 109.5 | O22—C25—C26 | 123.21 (19) |
| C24—C21—C22 | 109.65 (17) | O21—C25—C26 | 116.51 (19) |
| C24—C21—C23 | 110.46 (18) | C25—C26—H26A | 109.5 |
| C22—C21—C23 | 110.65 (17) | C25—C26—H26B | 109.5 |
| C24—C21—Sn1 | 109.79 (13) | H26A—C26—H26B | 109.5 |
| C22—C21—Sn1 | 110.17 (14) | C25—C26—H26C | 109.5 |
| C23—C21—Sn1 | 106.07 (13) | H26A—C26—H26C | 109.5 |
| C21—C22—H22A | 109.5 | H26B—C26—H26C | 109.5 |
| | | | |

Hydrogen-bond geometry (Å, °)

| D—H···A | <i>D</i> —Н | H···A | D····A | D—H···A |
|--------------------------------------|-------------|-------|-----------|---------|
| C12—H12C···O21 ⁱ | 0.98 | 2.54 | 3.362 (3) | 142 |
| C22—H22 <i>C</i> ···O11 ⁱ | 0.98 | 2.65 | 3.584 (3) | 160 |

| | | | supporting information | |
|---------------------------------|------|------|------------------------|-----|
| C16—H16C····O22 ⁱⁱ | 0.98 | 2.69 | 3.636 (3) | 163 |
| C16—H16A····O22 ⁱⁱⁱⁱ | 0.98 | 2.60 | 3.518 (3) | 155 |

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