# metal-organic compounds

# [2-(1,3-Dithiolan-2-ylidene)-5-(4-methylphenyl)-3-oxopent-4-enoato-$\kappa O$]triphenyltin(IV)

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In the title compound, $[Sn(C_6H_5)_3(C_{17}H_{17}O_3S_2)]$, the $Sn^{IV}$ atom adopts a distorted tetrahedral $SnC_3O$ geometry. A short intramolecular Sn···O contact of 2.793 (2) Å also occurs.

## Related literature

For related literature, see: James *et al.* (1992).
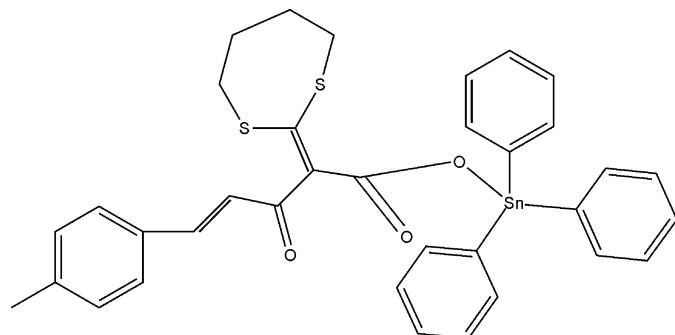
# Experimental

## Crystal data

| | |
|---|---|
| $[Sn(C_6H_5)_3(C_{17}H_{17}O_3S_2)]$ | $V$ = 3230.4 (11) Å$^3$ |
| $M_r$ = 683.42 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a$ = 12.736 (3) Å | $\mu$ = 0.95 mm$^{-1}$ |
| $b$ = 14.945 (3) Å | $T$ = 292 (2) K |
| $c$ = 17.733 (4) Å | $0.43 \times 0.21 \times 0.08$ mm |
| $\beta$ = 106.85 (3)° | |

## Data collection

| | |
|---|---|
| Bruker APEX diffractometer | 7230 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2002) | 5654 independent reflections |
| | 4186 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.793, $T_{max}$ = 0.943 | $R_{int}$ = 0.017 |

## Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.029 | 370 parameters |
| $wR(F^2)$ = 0.066 | H-atom parameters constrained |
| $S$ = 0.91 | $\Delta\rho_{max}$ = 0.32 e Å$^{-3}$ |
| 5654 reflections | $\Delta\rho_{min}$ = −0.25 e Å$^{-3}$ |

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

| | | | |
|---|---|---|---|
| Sn—O1 | 2.0716 (19) | Sn—C1 | 2.128 (3) |
| Sn—C13 | 2.121 (3) | Sn—C7 | 2.135 (3) |

Data collection: *SMART* (Bruker, 2002); 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); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2734).

## References

Bruker (2002). *SMART, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

James, B. D., Gioskos, S., Chandra, S., Magee, R. J. & Cashion, J. D. (1992). *J. Organomet. Chem.* **436**, 155–167.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

# [2-(1,3-Dithiolan-2-ylidene)-5-(4-methylphenyl)-3-oxopent-4-enoato-*κO*]triphenyltin(IV)

## Ze-Min Mei and Wei Fang

### S1. Comment

Organotin compounds have been extensively studied owing their biological activities and varied structures (e.g. James *et al.*, 1992). Here, we present the synthesis and structure of the title molecular complex, (I), (Fig. 1).

The tin atom in (I) is coordinated to three carbon atoms from three phenyl groups and one oxygen atom from a carboxylate group (Table 1). A short Sn···O contact of 2.793 (2)Å also occurs, so the coordination of the carboxylate group could also be described as very asymmetric bidentate although the C-O bond lengths are very different [1.224 (3) and 1.300 (3)Å], suggestive of charge localisation.

### S2. Experimental

A mixture of Ph$_3$SnOH (1.0 mmol) and 2-[1,3]dithiolan-2-ylidene-3-oxo-5-(4-methelphenyl)-pent-4-enolic acid 2 (1.0 mmol) in toluene (20 ml) was refluxed for 3 h and water released in the reaction was removed azeotropically by a Dean-Stark apparatus. The reaction mixture was then cooled and toluene removed by a rotary evaporator. The resulting solid product was recrystallized with ethanol to give colourless slabs of (I).

### S3. Refinement

All H atoms were placed geometrically (C—H = 0.93-0.97 Å) and refined as riding with $U_{iso}$(H) fixed at 0.08Å$^2$.
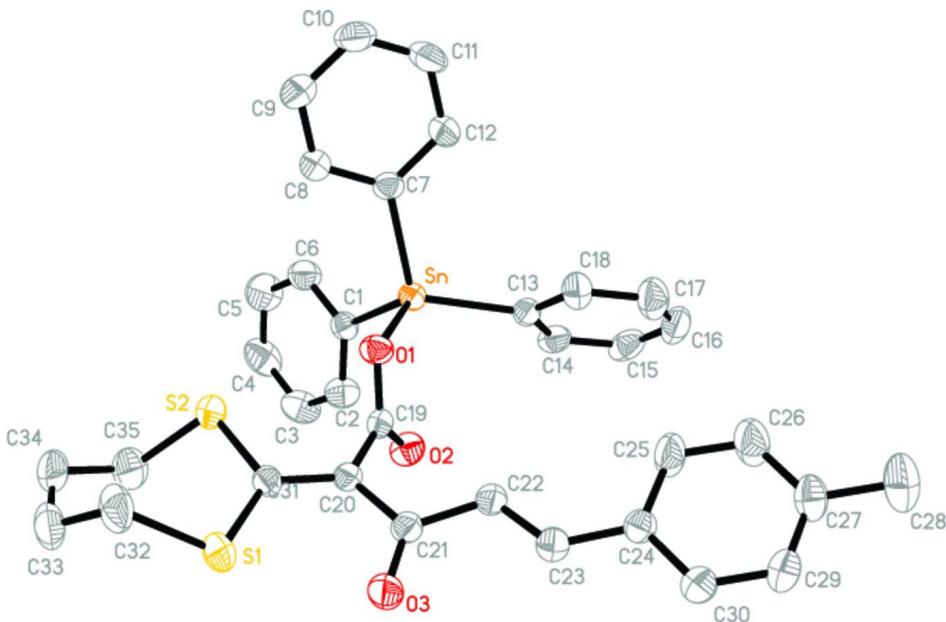
**Figure 1**

The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level (H atoms omitted for clarity).

**[2-(1,3-Dithiolan-2-ylidene)-5-(4-methylphenyl)-3-oxopent-4-enoato- *κ*O]triphenyltin(IV)**

*Crystal data*
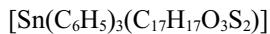
| | |
|---|---|
| [Sn(C$_6$H$_5$)$_3$(C$_{17}$H$_{17}$O$_3$S$_2$)] | $Z = 4$ |
| $M_r = 683.42$ | $F(000) = 1392$ |
| Monoclinic, $P2_1/c$ | $D_x = 1.405$ Mg m$^{-3}$ |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 12.736$ (3) Å | $\theta = 2.9$–22.2° |
| $b = 14.945$ (3) Å | $\mu = 0.95$ mm$^{-1}$ |
| $c = 17.733$ (4) Å | $T = 292$ K |
| $\beta = 106.85$ (3)° | Slab, colourless |
| $V = 3230.4$ (11) Å$^3$ | $0.43 \times 0.21 \times 0.08$ mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII diffractometer | 7230 measured reflections |
| Radiation source: fine-focus sealed tube | 5654 independent reflections |
| Graphite monochromator | 4186 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 0 pixels mm$^{-1}$ | $R_{int} = 0.017$ |
| $\omega$ scans | $\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$ |
| Absorption correction: multi-scan | $h = -1 \rightarrow 15$ |
| (*SADABS*; Bruker, 2002) | $k = -1 \rightarrow 17$ |
| $T_{min} = 0.793$, $T_{max} = 0.943$ | $l = -21 \rightarrow 20$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | 5654 reflections |
| Least-squares matrix: full | 370 parameters |
| $R[F^2 > 2\sigma(F^2)] = 0.029$ | 0 restraints |
| $wR(F^2) = 0.066$ | Primary atom site location: structure-invariant |
| $S = 0.91$ | direct methods |

| | |
|---|---|
| Secondary atom site location: difference Fourier map | $w = 1/[\sigma^2(F_o^2) + (0.0285P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Hydrogen site location: inferred from neighbouring sites | $(\Delta/\sigma)_{max} = 0.001$ |
| H-atom parameters constrained | $\Delta\rho_{max} = 0.32$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.25$ e Å$^{-3}$ |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Sn | 0.369434 (16) | 0.896438 (14) | 0.055072 (11) | 0.04525 (7) |
| S1 | 0.04717 (8) | 0.68154 (7) | 0.23041 (5) | 0.0680 (2) |
| S2 | 0.16556 (7) | 0.85632 (6) | 0.21982 (5) | 0.0676 (2) |
| O1 | 0.31329 (16) | 0.80230 (14) | 0.11995 (11) | 0.0529 (5) |
| O2 | 0.16982 (18) | 0.80468 (14) | 0.01464 (12) | 0.0605 (6) |
| O3 | 0.0657 (2) | 0.57848 (15) | 0.10596 (15) | 0.0754 (7) |
| C1 | 0.2679 (2) | 1.0122 (2) | 0.03678 (16) | 0.0480 (7) |
| C2 | 0.1598 (3) | 1.0121 (2) | −0.0094 (2) | 0.0654 (9) |
| H2 | 0.1293 | 0.9594 | −0.0342 | 0.080* |
| C3 | 0.0962 (3) | 1.0882 (3) | −0.0197 (2) | 0.0789 (11) |
| H3 | 0.0234 | 1.0865 | −0.0504 | 0.080* |
| C4 | 0.1402 (4) | 1.1657 (3) | 0.0153 (3) | 0.0890 (13) |
| H4 | 0.0976 | 1.2173 | 0.0086 | 0.080* |
| C5 | 0.2478 (4) | 1.1680 (3) | 0.0608 (3) | 0.0944 (13) |
| H5 | 0.2777 | 1.2212 | 0.0849 | 0.080* |
| C6 | 0.3114 (3) | 1.0923 (2) | 0.0708 (2) | 0.0677 (9) |
| H6 | 0.3845 | 1.0949 | 0.1009 | 0.080* |
| C7 | 0.5206 (2) | 0.91750 (19) | 0.14472 (18) | 0.0491 (7) |
| C8 | 0.5215 (3) | 0.9442 (2) | 0.22032 (18) | 0.0599 (8) |
| H8 | 0.4553 | 0.9551 | 0.2310 | 0.080* |
| C9 | 0.6177 (3) | 0.9546 (3) | 0.2790 (2) | 0.0757 (11) |
| H9 | 0.6164 | 0.9723 | 0.3291 | 0.080* |
| C10 | 0.7161 (3) | 0.9392 (3) | 0.2644 (2) | 0.0787 (11) |
| H10 | 0.7814 | 0.9470 | 0.3042 | 0.080* |
| C11 | 0.7180 (3) | 0.9124 (3) | 0.1916 (2) | 0.0786 (11) |
| H11 | 0.7849 | 0.9013 | 0.1821 | 0.080* |
| C12 | 0.6215 (2) | 0.9013 (2) | 0.13137 (19) | 0.0602 (8) |
| H12 | 0.6240 | 0.8831 | 0.0818 | 0.080* |
| C13 | 0.3984 (2) | 0.8288 (2) | −0.04210 (16) | 0.0473 (7) |
| C14 | 0.3547 (3) | 0.8590 (2) | −0.11887 (18) | 0.0596 (8) |

| | | | |
|---|---|---|---|
| H14 | 0.3090 | 0.9088 | −0.1289 | 0.080* |
| C15 | 0.3792 (3) | 0.8153 (3) | −0.18026 (19) | 0.0758 (11) |
| H15 | 0.3493 | 0.8357 | −0.2316 | 0.080* |
| C16 | 0.4463 (4) | 0.7428 (3) | −0.1666 (3) | 0.0853 (13) |
| H16 | 0.4633 | 0.7148 | −0.2084 | 0.080* |
| C17 | 0.4890 (4) | 0.7108 (3) | −0.0920 (3) | 0.0829 (12) |
| H17 | 0.5331 | 0.6600 | −0.0831 | 0.080* |
| C18 | 0.4665 (3) | 0.7542 (2) | −0.0297 (2) | 0.0651 (9) |
| H18 | 0.4973 | 0.7332 | 0.0213 | 0.080* |
| C19 | 0.2141 (2) | 0.77828 (19) | 0.08166 (17) | 0.0452 (7) |
| C20 | 0.1567 (2) | 0.71697 (19) | 0.12296 (15) | 0.0436 (7) |
| C21 | 0.1364 (2) | 0.62483 (19) | 0.09161 (17) | 0.0494 (7) |
| C22 | 0.2053 (3) | 0.59116 (19) | 0.04431 (17) | 0.0503 (7) |
| H22 | 0.2623 | 0.6267 | 0.0383 | 0.080* |
| C23 | 0.1887 (3) | 0.5114 (2) | 0.00984 (17) | 0.0522 (7) |
| H23 | 0.1314 | 0.4781 | 0.0183 | 0.080* |
| C24 | 0.2480 (2) | 0.4690 (2) | −0.03935 (17) | 0.0502 (7) |
| C25 | 0.3373 (3) | 0.5064 (2) | −0.0554 (2) | 0.0894 (13) |
| H25 | 0.3645 | 0.5608 | −0.0323 | 0.080* |
| C26 | 0.3877 (4) | 0.4655 (3) | −0.1050 (3) | 0.1033 (16) |
| H26 | 0.4478 | 0.4935 | −0.1145 | 0.080* |
| C27 | 0.3535 (3) | 0.3857 (2) | −0.1407 (2) | 0.0694 (10) |
| C28 | 0.4098 (4) | 0.3420 (3) | −0.1948 (2) | 0.1017 (15) |
| H28A | 0.4700 | 0.3787 | −0.1985 | 0.080* |
| H28B | 0.3585 | 0.3352 | −0.2462 | 0.080* |
| H28C | 0.4367 | 0.2843 | −0.1744 | 0.080* |
| C29 | 0.2650 (3) | 0.3485 (3) | −0.1252 (2) | 0.0863 (12) |
| H29 | 0.2381 | 0.2943 | −0.1488 | 0.080* |
| C30 | 0.2133 (3) | 0.3887 (2) | −0.0754 (2) | 0.0753 (10) |
| H30 | 0.1533 | 0.3605 | −0.0660 | 0.080* |
| C31 | 0.1233 (2) | 0.7476 (2) | 0.18458 (15) | 0.0476 (7) |
| C32 | 0.0722 (3) | 0.7268 (3) | 0.32917 (18) | 0.0852 (12) |
| H32A | 0.0642 | 0.6786 | 0.3637 | 0.080* |
| H32B | 0.1478 | 0.7468 | 0.3471 | 0.080* |
| C33 | −0.0004 (3) | 0.8036 (3) | 0.3391 (2) | 0.0883 (13) |
| H33A | −0.0742 | 0.7930 | 0.3054 | 0.080* |
| H33B | −0.0035 | 0.8038 | 0.3932 | 0.080* |
| C34 | 0.0353 (4) | 0.8927 (3) | 0.3209 (2) | 0.0983 (15) |
| H34A | 0.1061 | 0.9054 | 0.3582 | 0.080* |
| H34B | −0.0162 | 0.9366 | 0.3294 | 0.080* |
| C35 | 0.0451 (3) | 0.9053 (3) | 0.2383 (2) | 0.0832 (12) |
| H35A | 0.0450 | 0.9690 | 0.2276 | 0.080* |
| H35B | −0.0195 | 0.8798 | 0.2012 | 0.080* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sn | 0.04499 (11) | 0.04695 (12) | 0.04510 (11) | −0.00348 (11) | 0.01511 (8) | −0.00145 (10) |

| | | | | | |
|---|---|---|---|---|---|
| S1 | 0.0732 (6) | 0.0831 (6) | 0.0592 (5) | −0.0096 (5) | 0.0375 (4) | −0.0034 (5) |
| S2 | 0.0619 (5) | 0.0686 (6) | 0.0770 (6) | −0.0067 (5) | 0.0276 (5) | −0.0286 (5) |
| O1 | 0.0483 (12) | 0.0601 (13) | 0.0505 (11) | −0.0097 (11) | 0.0145 (10) | 0.0038 (10) |
| O2 | 0.0680 (14) | 0.0639 (14) | 0.0470 (12) | −0.0052 (12) | 0.0125 (11) | 0.0064 (11) |
| O3 | 0.0801 (17) | 0.0673 (16) | 0.0954 (18) | −0.0277 (13) | 0.0517 (15) | −0.0229 (13) |
| C1 | 0.0501 (18) | 0.0473 (18) | 0.0500 (16) | −0.0004 (15) | 0.0199 (15) | 0.0040 (14) |
| C2 | 0.060 (2) | 0.062 (2) | 0.069 (2) | 0.0024 (19) | 0.0090 (18) | 0.0082 (18) |
| C3 | 0.062 (2) | 0.078 (3) | 0.093 (3) | 0.008 (2) | 0.017 (2) | 0.024 (2) |
| C4 | 0.078 (3) | 0.067 (3) | 0.129 (4) | 0.024 (2) | 0.042 (3) | 0.016 (3) |
| C5 | 0.097 (3) | 0.054 (2) | 0.134 (4) | 0.005 (2) | 0.036 (3) | −0.015 (2) |
| C6 | 0.057 (2) | 0.062 (2) | 0.082 (2) | −0.0036 (19) | 0.0177 (18) | −0.0059 (19) |
| C7 | 0.0453 (17) | 0.0444 (18) | 0.0567 (17) | −0.0069 (14) | 0.0134 (14) | −0.0024 (14) |
| C8 | 0.0530 (19) | 0.069 (2) | 0.0597 (19) | −0.0056 (18) | 0.0192 (16) | −0.0092 (17) |
| C9 | 0.070 (2) | 0.093 (3) | 0.059 (2) | −0.010 (2) | 0.0114 (19) | −0.014 (2) |
| C10 | 0.054 (2) | 0.090 (3) | 0.080 (3) | −0.008 (2) | −0.0017 (19) | −0.008 (2) |
| C11 | 0.0416 (19) | 0.093 (3) | 0.101 (3) | 0.003 (2) | 0.0200 (19) | −0.005 (2) |
| C12 | 0.0523 (18) | 0.066 (2) | 0.068 (2) | −0.0056 (18) | 0.0252 (16) | −0.0061 (18) |
| C13 | 0.0487 (17) | 0.0497 (17) | 0.0466 (16) | −0.0084 (15) | 0.0190 (14) | −0.0039 (14) |
| C14 | 0.0555 (19) | 0.067 (2) | 0.0544 (18) | −0.0163 (18) | 0.0127 (16) | −0.0024 (16) |
| C15 | 0.088 (3) | 0.094 (3) | 0.0456 (18) | −0.037 (3) | 0.0198 (19) | −0.011 (2) |
| C16 | 0.110 (3) | 0.080 (3) | 0.088 (3) | −0.041 (3) | 0.063 (3) | −0.038 (2) |
| C17 | 0.101 (3) | 0.057 (2) | 0.108 (3) | −0.004 (2) | 0.058 (3) | −0.015 (2) |
| C18 | 0.075 (2) | 0.062 (2) | 0.065 (2) | 0.0032 (19) | 0.0303 (19) | −0.0027 (18) |
| C19 | 0.0487 (17) | 0.0416 (16) | 0.0477 (17) | −0.0021 (14) | 0.0178 (14) | −0.0101 (14) |
| C20 | 0.0422 (16) | 0.0498 (17) | 0.0384 (14) | −0.0042 (14) | 0.0112 (12) | −0.0032 (13) |
| C21 | 0.0512 (17) | 0.0511 (19) | 0.0469 (16) | −0.0062 (15) | 0.0159 (14) | −0.0015 (13) |
| C22 | 0.0530 (18) | 0.0492 (19) | 0.0521 (16) | −0.0087 (15) | 0.0206 (14) | −0.0047 (14) |
| C23 | 0.0559 (19) | 0.0492 (18) | 0.0525 (17) | −0.0004 (16) | 0.0173 (15) | 0.0018 (15) |
| C24 | 0.0541 (18) | 0.0438 (17) | 0.0527 (17) | 0.0005 (15) | 0.0155 (15) | 0.0005 (14) |
| C25 | 0.116 (3) | 0.059 (2) | 0.123 (3) | −0.029 (2) | 0.080 (3) | −0.037 (2) |
| C26 | 0.124 (4) | 0.074 (3) | 0.149 (4) | −0.026 (3) | 0.099 (3) | −0.027 (3) |
| C27 | 0.093 (3) | 0.057 (2) | 0.068 (2) | 0.017 (2) | 0.039 (2) | 0.0083 (18) |
| C28 | 0.152 (4) | 0.080 (3) | 0.099 (3) | 0.025 (3) | 0.076 (3) | 0.009 (2) |
| C29 | 0.089 (3) | 0.070 (3) | 0.104 (3) | −0.001 (2) | 0.034 (3) | −0.035 (2) |
| C30 | 0.067 (2) | 0.063 (2) | 0.101 (3) | −0.009 (2) | 0.032 (2) | −0.022 (2) |
| C31 | 0.0419 (16) | 0.0578 (18) | 0.0433 (15) | 0.0030 (14) | 0.0124 (13) | −0.0024 (14) |
| C32 | 0.085 (3) | 0.131 (4) | 0.0451 (18) | 0.018 (3) | 0.0262 (18) | 0.007 (2) |
| C33 | 0.076 (3) | 0.136 (4) | 0.059 (2) | 0.022 (3) | 0.030 (2) | −0.014 (3) |
| C34 | 0.077 (3) | 0.130 (4) | 0.093 (3) | 0.008 (3) | 0.033 (2) | −0.053 (3) |
| C35 | 0.079 (3) | 0.074 (3) | 0.099 (3) | 0.019 (2) | 0.031 (2) | −0.017 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Sn—O1 | 2.0716 (19) | C16—C17 | 1.362 (5) |
| Sn—C13 | 2.121 (3) | C16—H16 | 0.9300 |
| Sn—C1 | 2.128 (3) | C17—C18 | 1.381 (4) |
| Sn—C7 | 2.135 (3) | C17—H17 | 0.9300 |
| S1—C31 | 1.741 (3) | C18—H18 | 0.9300 |

| | | | |
|---|---|---|---|
| S1—C32 | 1.817 (3) | C19—C20 | 1.490 (4) |
| S2—C31 | 1.768 (3) | C20—C31 | 1.361 (4) |
| S2—C35 | 1.813 (3) | C20—C21 | 1.479 (4) |
| C19—O1 | 1.300 (3) | C21—C22 | 1.468 (4) |
| C19—O2 | 1.224 (3) | C22—C23 | 1.329 (4) |
| C21—O3 | 1.219 (3) | C22—H22 | 0.9300 |
| C1—C6 | 1.381 (4) | C23—C24 | 1.454 (4) |
| C1—C2 | 1.383 (4) | C23—H23 | 0.9300 |
| C2—C3 | 1.378 (5) | C24—C25 | 1.370 (4) |
| C2—H2 | 0.9300 | C24—C30 | 1.371 (4) |
| C3—C4 | 1.356 (5) | C25—C26 | 1.372 (5) |
| C3—H3 | 0.9300 | C25—H25 | 0.9300 |
| C4—C5 | 1.374 (6) | C26—C27 | 1.361 (5) |
| C4—H4 | 0.9300 | C26—H26 | 0.9300 |
| C5—C6 | 1.374 (5) | C27—C29 | 1.356 (5) |
| C5—H5 | 0.9300 | C27—C28 | 1.504 (5) |
| C6—H6 | 0.9300 | C28—H28A | 0.9600 |
| C7—C12 | 1.393 (4) | C28—H28B | 0.9600 |
| C7—C8 | 1.395 (4) | C28—H28C | 0.9600 |
| C8—C9 | 1.368 (4) | C29—C30 | 1.382 (5) |
| C8—H8 | 0.9300 | C29—H29 | 0.9300 |
| C9—C10 | 1.371 (5) | C30—H30 | 0.9300 |
| C9—H9 | 0.9300 | C32—C33 | 1.516 (5) |
| C10—C11 | 1.358 (5) | C32—H32A | 0.9700 |
| C10—H10 | 0.9300 | C32—H32B | 0.9700 |
| C11—C12 | 1.385 (5) | C33—C34 | 1.472 (5) |
| C11—H11 | 0.9300 | C33—H33A | 0.9700 |
| C12—H12 | 0.9300 | C33—H33B | 0.9700 |
| C13—C14 | 1.389 (4) | C34—C35 | 1.519 (5) |
| C13—C18 | 1.390 (4) | C34—H34A | 0.9700 |
| C14—C15 | 1.380 (5) | C34—H34B | 0.9700 |
| C14—H14 | 0.9300 | C35—H35A | 0.9700 |
| C15—C16 | 1.359 (5) | C35—H35B | 0.9700 |
| C15—H15 | 0.9300 | | |
| | | | |
| O1—Sn—C13 | 107.27 (10) | O1—C19—C20 | 117.0 (2) |
| O1—Sn—C1 | 110.16 (9) | C31—C20—C21 | 123.6 (3) |
| C13—Sn—C1 | 120.34 (11) | C31—C20—C19 | 120.0 (3) |
| O1—Sn—C7 | 93.93 (9) | C21—C20—C19 | 116.4 (2) |
| C13—Sn—C7 | 110.09 (11) | O3—C21—C22 | 121.6 (3) |
| C1—Sn—C7 | 111.75 (11) | O3—C21—C20 | 120.6 (3) |
| C31—S1—C32 | 105.85 (17) | C22—C21—C20 | 117.7 (3) |
| C31—S2—C35 | 104.38 (17) | C23—C22—C21 | 121.9 (3) |
| C19—O1—Sn | 109.70 (17) | C23—C22—H22 | 119.0 |
| C6—C1—C2 | 117.7 (3) | C21—C22—H22 | 119.0 |
| C6—C1—Sn | 119.2 (2) | C22—C23—C24 | 128.7 (3) |
| C2—C1—Sn | 123.0 (2) | C22—C23—H23 | 115.6 |
| C3—C2—C1 | 121.5 (3) | C24—C23—H23 | 115.6 |

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| C3—C2—H2 | 119.3 | C25—C24—C30 | 115.8 (3) |
| C1—C2—H2 | 119.3 | C25—C24—C23 | 123.7 (3) |
| C4—C3—C2 | 119.7 (4) | C30—C24—C23 | 120.5 (3) |
| C4—C3—H3 | 120.1 | C24—C25—C26 | 121.5 (3) |
| C2—C3—H3 | 120.1 | C24—C25—H25 | 119.3 |
| C3—C4—C5 | 120.0 (4) | C26—C25—H25 | 119.3 |
| C3—C4—H4 | 120.0 | C27—C26—C25 | 122.9 (4) |
| C5—C4—H4 | 120.0 | C27—C26—H26 | 118.6 |
| C4—C5—C6 | 120.4 (4) | C25—C26—H26 | 118.6 |
| C4—C5—H5 | 119.8 | C29—C27—C26 | 116.0 (3) |
| C6—C5—H5 | 119.8 | C29—C27—C28 | 122.0 (4) |
| C5—C6—C1 | 120.6 (3) | C26—C27—C28 | 122.1 (4) |
| C5—C6—H6 | 119.7 | C27—C28—H28A | 109.5 |
| C1—C6—H6 | 119.7 | C27—C28—H28B | 109.5 |
| C12—C7—C8 | 117.5 (3) | H28A—C28—H28B | 109.5 |
| C12—C7—Sn | 121.6 (2) | C27—C28—H28C | 109.5 |
| C8—C7—Sn | 120.8 (2) | H28A—C28—H28C | 109.5 |
| C9—C8—C7 | 121.3 (3) | H28B—C28—H28C | 109.5 |
| C9—C8—H8 | 119.3 | C27—C29—C30 | 121.9 (4) |
| C7—C8—H8 | 119.3 | C27—C29—H29 | 119.0 |
| C8—C9—C10 | 120.2 (3) | C30—C29—H29 | 119.0 |
| C8—C9—H9 | 119.9 | C24—C30—C29 | 122.0 (4) |
| C10—C9—H9 | 119.9 | C24—C30—H30 | 119.0 |
| C11—C10—C9 | 119.9 (3) | C29—C30—H30 | 119.0 |
| C11—C10—H10 | 120.0 | C20—C31—S1 | 122.0 (2) |
| C9—C10—H10 | 120.0 | C20—C31—S2 | 117.3 (2) |
| C10—C11—C12 | 120.8 (3) | S1—C31—S2 | 120.63 (16) |
| C10—C11—H11 | 119.6 | C33—C32—S1 | 116.9 (3) |
| C12—C11—H11 | 119.6 | C33—C32—H32A | 108.1 |
| C11—C12—C7 | 120.3 (3) | S1—C32—H32A | 108.1 |
| C11—C12—H12 | 119.9 | C33—C32—H32B | 108.1 |
| C7—C12—H12 | 119.9 | S1—C32—H32B | 108.1 |
| C14—C13—C18 | 118.0 (3) | H32A—C32—H32B | 107.3 |
| C14—C13—Sn | 121.8 (2) | C34—C33—C32 | 114.9 (3) |
| C18—C13—Sn | 120.1 (2) | C34—C33—H33A | 108.5 |
| C15—C14—C13 | 120.1 (3) | C32—C33—H33A | 108.5 |
| C15—C14—H14 | 120.0 | C34—C33—H33B | 108.5 |
| C13—C14—H14 | 120.0 | C32—C33—H33B | 108.5 |
| C16—C15—C14 | 120.8 (3) | H33A—C33—H33B | 107.5 |
| C16—C15—H15 | 119.6 | C33—C34—C35 | 116.2 (3) |
| C14—C15—H15 | 119.6 | C33—C34—H34A | 108.2 |
| C15—C16—C17 | 120.4 (4) | C35—C34—H34A | 108.2 |
| C15—C16—H16 | 119.8 | C33—C34—H34B | 108.2 |
| C17—C16—H16 | 119.8 | C35—C34—H34B | 108.2 |
| C16—C17—C18 | 119.7 (4) | H34A—C34—H34B | 107.4 |
| C16—C17—H17 | 120.2 | C34—C35—S2 | 115.8 (3) |
| C18—C17—H17 | 120.2 | C34—C35—H35A | 108.3 |
| C17—C18—C13 | 121.0 (3) | S2—C35—H35A | 108.3 |

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| C17—C18—H18 | 119.5 | C34—C35—H35B | 108.3 |
| C13—C18—H18 | 119.5 | S2—C35—H35B | 108.3 |
| O2—C19—O1 | 121.5 (3) | H35A—C35—H35B | 107.4 |
| O2—C19—C20 | 121.5 (3) | | |
| | | | |
| C13—Sn—O1—C19 | −71.56 (19) | C16—C17—C18—C13 | 1.7 (5) |
| C1—Sn—O1—C19 | 61.1 (2) | C14—C13—C18—C17 | −0.7 (5) |
| C7—Sn—O1—C19 | 175.99 (18) | Sn—C13—C18—C17 | −178.1 (3) |
| O1—Sn—C1—C6 | 114.2 (2) | Sn—O1—C19—O2 | 5.6 (3) |
| C13—Sn—C1—C6 | −120.2 (2) | Sn—O1—C19—C20 | −174.50 (19) |
| C7—Sn—C1—C6 | 11.2 (3) | O2—C19—C20—C31 | −109.5 (3) |
| O1—Sn—C1—C2 | −67.2 (3) | O1—C19—C20—C31 | 70.6 (4) |
| C13—Sn—C1—C2 | 58.3 (3) | O2—C19—C20—C21 | 68.6 (4) |
| C7—Sn—C1—C2 | −170.2 (2) | O1—C19—C20—C21 | −111.2 (3) |
| C6—C1—C2—C3 | −1.8 (5) | C31—C20—C21—O3 | 18.6 (5) |
| Sn—C1—C2—C3 | 179.6 (3) | C19—C20—C21—O3 | −159.5 (3) |
| C1—C2—C3—C4 | 0.9 (6) | C31—C20—C21—C22 | −160.3 (3) |
| C2—C3—C4—C5 | −0.1 (6) | C19—C20—C21—C22 | 21.6 (4) |
| C3—C4—C5—C6 | 0.3 (7) | O3—C21—C22—C23 | 5.3 (5) |
| C4—C5—C6—C1 | −1.3 (6) | C20—C21—C22—C23 | −175.9 (3) |
| C2—C1—C6—C5 | 2.0 (5) | C21—C22—C23—C24 | 179.1 (3) |
| Sn—C1—C6—C5 | −179.4 (3) | C22—C23—C24—C25 | 2.8 (5) |
| O1—Sn—C7—C12 | 120.0 (3) | C22—C23—C24—C30 | −174.6 (3) |
| C13—Sn—C7—C12 | 10.0 (3) | C30—C24—C25—C26 | 0.3 (6) |
| C1—Sn—C7—C12 | −126.5 (3) | C23—C24—C25—C26 | −177.2 (4) |
| O1—Sn—C7—C8 | −57.0 (3) | C24—C25—C26—C27 | −0.5 (7) |
| C13—Sn—C7—C8 | −167.0 (2) | C25—C26—C27—C29 | 0.6 (7) |
| C1—Sn—C7—C8 | 56.5 (3) | C25—C26—C27—C28 | 180.0 (4) |
| C12—C7—C8—C9 | 0.4 (5) | C26—C27—C29—C30 | −0.7 (6) |
| Sn—C7—C8—C9 | 177.5 (3) | C28—C27—C29—C30 | 180.0 (4) |
| C7—C8—C9—C10 | 0.2 (6) | C25—C24—C30—C29 | −0.4 (6) |
| C8—C9—C10—C11 | −0.8 (7) | C23—C24—C30—C29 | 177.2 (3) |
| C9—C10—C11—C12 | 0.8 (6) | C27—C29—C30—C24 | 0.7 (6) |
| C10—C11—C12—C7 | −0.2 (6) | C21—C20—C31—S1 | −2.8 (4) |
| C8—C7—C12—C11 | −0.4 (5) | C19—C20—C31—S1 | 175.2 (2) |
| Sn—C7—C12—C11 | −177.5 (3) | C21—C20—C31—S2 | 174.4 (2) |
| O1—Sn—C13—C14 | 128.4 (2) | C19—C20—C31—S2 | −7.6 (4) |
| C1—Sn—C13—C14 | 1.6 (3) | C32—S1—C31—C20 | 156.1 (2) |
| C7—Sn—C13—C14 | −130.6 (2) | C32—S1—C31—S2 | −21.1 (2) |
| O1—Sn—C13—C18 | −54.3 (3) | C35—S2—C31—C20 | 138.4 (2) |
| C1—Sn—C13—C18 | 178.8 (2) | C35—S2—C31—S1 | −44.3 (2) |
| C7—Sn—C13—C18 | 46.6 (3) | C31—S1—C32—C33 | 86.2 (3) |
| C18—C13—C14—C15 | 0.1 (5) | S1—C32—C33—C34 | −83.9 (4) |
| Sn—C13—C14—C15 | 177.3 (2) | C32—C33—C34—C35 | 58.3 (5) |
| C13—C14—C15—C16 | −0.4 (5) | C33—C34—C35—S2 | −76.7 (4) |
| C14—C15—C16—C17 | 1.4 (6) | C31—S2—C35—C34 | 91.1 (3) |
| C15—C16—C17—C18 | −2.0 (6) | | |