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(2-Chloro-4-nitrobenzoato)(methanol)-triphenyltin(IV)

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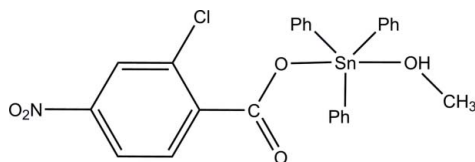
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.024; wR factor = 0.060; data-to-parameter ratio = 33.5.

In the title complex, $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_7\text{H}_3\text{ClNO}_4)(\text{CH}_4\text{O})]$, the five-coordinate Sn^{IV} atom exists in a trigonal-bipyramidal environment, formed by a monodentate carboxylate group, three phenyl rings and a methanol molecule. The axial sites are occupied by the O atoms of the methanol molecule and the carboxylate group, while the equatorial plane is formed by the C atoms of three phenyl rings. The benzene ring of the 2-chloro-4-nitrobenzoate ligand makes dihedral angles of $66.18(7)$, $74.71(7)$ and $77.39(7)^\circ$ with respect to the three phenyl rings. In the crystal, the molecules are linked *via* intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds into a column along the b axis.

Related literature

For general background to and the coordination environment of the title complex, see: Yeap & Teoh (2003); Szorcik *et al.* (2006); Álvarez-Boo *et al.* (2006). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_7\text{H}_3\text{ClNO}_4)(\text{CH}_4\text{O})]$
 $M_r = 582.59$

 Monoclinic, $P2_1/c$
 $a = 9.0287(3)$ Å

 $b = 13.5239(4)$ Å
 $c = 20.7505(6)$ Å
 $\beta = 108.894(1)^\circ$
 $V = 2397.19(13)$ Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 1.22$ mm⁻¹
 $T = 100$ K
 $0.27 \times 0.25 \times 0.15$ mm

Data collection

 Bruker SMART APEXII DUO
 CCD area-detector
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\text{min}} = 0.739$, $T_{\text{max}} = 0.835$

 42634 measured reflections
 10460 independent reflections
 9263 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.060$
 $S = 1.04$
 10460 reflections
 312 parameters

 H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{\text{max}} = 2.82$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H1O3}\cdots\text{O2}^i$	0.79 (3)	1.83 (3)	2.6082 (14)	170 (3)
$\text{C16}-\text{H16A}\cdots\text{O4}^{ii}$	0.93	2.58	3.312 (2)	136

Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x, y + 1, z$.

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2695).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Álvarez-Boo, P., Casas, J. S., Couce, M. D., Farto, R., Fernández-Moreira, V., Freijanes, E., Sordo, J. & Vázquez-López, E. (2006). *J. Organomet. Chem.* **691**, 45–52.
- Bruker (2009). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Szorcik, A., Nagy, L., Scopelliti, M., Deák, A., Pellerito, L., Galbács, G. & Hered, M. (2006). *J. Organomet. Chem.* **691**, 1622–1630.
- Yeap, L.-L. & Teoh, S.-G. (2003). *J. Coord. Chem.* **56**, 701–708.

‡ Thomson Reuters ResearcherID: A-5525-2009.

§ Thomson Reuters ResearcherID: A-3561-2009.

supplementary materials

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(2-Chloro-4-nitrobenzoato)(methanol)triphenyltin(IV)

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Comment

There are a number of well documented literature indicating triphenyltin(IV) carboxylate complexes existing in monomeric five-coordinated structures, e.g. in structures in which the carboxylate anion is bonded to the tin(IV) atom in a monodentate mode and extra coordination being contributed from the coordinating ligands (Yeap & Teoh, 2003; Szorcik *et al.*, 2006; Álvarez-Boo *et al.*, 2006). The coordinating ligands may be derivatives of coordinating solvents or from pyridine derivatives or amine. Complex (2,6-difluorobenzoato)triphenyltin(IV) showed that the two fluorine atoms at the ortho positions of the benzene fragment while the ethanol molecule was attached to the tin(IV) atom resulting the tin(IV) atom being five-coordinated (Yeap & Teoh, 2003).

The structure of the titled complex (Fig. 1) is similar to (2,6-difluorobenzoato)triphenyltin(IV). The only difference is that the methanol molecule participated in the crystal structure. In the title complex, the five-coordinate tin(IV) (Sn1) atom exists in a trigonal-bipyramidal environment, formed by a monodentate carboxylate group, three phenyl rings and a coordinated methanol molecule. The axial sites are occupied by the O atoms of the methanol and carboxylate [O1—Sn1—O3 = 169.05 (3)°], with the three phenyl rings occupying the equatorial plane. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The benzene ring (C20—C25) of 2-chloro-4-nitrobenzoate ligand makes dihedral angles of 66.18 (7), 74.71 (7) and 77.39 (7)° with respect to the three phenyl rings (C1—C6, C7—C12 and C13—C18). In the crystal structure, the molecules are linked *via* intermolecular O3—H1O3...O2 and C16—H16A...O4 hydrogen bonds (Table 1) into a column along the *b* axis (Fig. 2).

Experimental

The title complex was obtained by heating under reflux a 1:1 molar mixture of triphenyltin(IV) hydroxide (1.10 g, 3 mmol) and 2-chloro-4-nitrobenzoic acid (0.60 g, 3 mmol) in methanol (50 mL) for 2 h. A clear transparent solution was isolated by filtration and kept in a bottle. After a few days, crystals (1.36 g, 78.2 % yield) were collected (*m.p.*: 119.0–120.0 °C). Analysis for C₂₆H₂₂NO₅ClSn: C 53.45, H 3.74, N 2.34%. Calculated for C₂₆H₂₂NO₅ClSn: C 53.60, H 3.81, N 2.40%.

Refinement

H1O3 was located in a difference Fourier map and allowed to refined freely. The remaining H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 or 0.96 Å and $U_{iso}(H) = 1.2$ or $1.5 U_{eq}(C)$. A rotating-group model was applied for the methyl group. The highest residual electron density peak and the deepest hole are located at 0.57 and 0.53 Å, respectively, from atom Sn1.

Figures

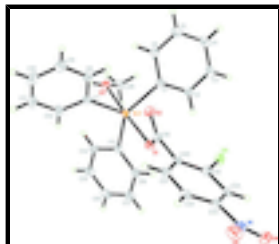


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids for non-H atoms.

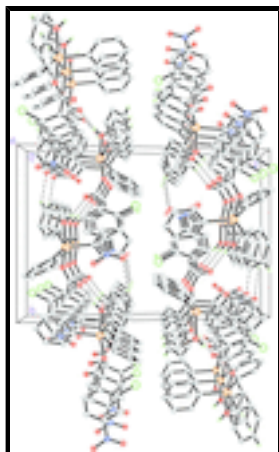


Fig. 2. Packing diagram of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

(2-Chloro-4-nitrobenzoato)(methanol)triphenyltin(IV)

Crystal data

[Sn(C₆H₅)₃(C₇H₃ClNO₄)(CH₄O)]

M_r = 582.59

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 9.0287 (3) Å

b = 13.5239 (4) Å

c = 20.7505 (6) Å

β = 108.894 (1)°

V = 2397.19 (13) Å³

Z = 4

F(000) = 1168

D_x = 1.614 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 9909 reflections

θ = 3.7–37.5°

μ = 1.22 mm⁻¹

T = 100 K

Block, yellow

0.27 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEXII DUO CCD area-detector diffractometer

10460 independent reflections

Radiation source: fine-focus sealed tube graphite

9263 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.023

φ and ω scans

θ_{max} = 35.0°, θ_{min} = 1.8°

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)

h = -14→13

$T_{\min} = 0.739$, $T_{\max} = 0.835$
42634 measured reflections

$k = -21 \rightarrow 21$
 $l = -33 \rightarrow 33$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.060$

$S = 1.04$

10460 reflections

312 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

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 1.8694P]$

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

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

$\Delta\rho_{\max} = 2.82 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -1.27 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.122653 (9)	0.424304 (6)	0.818254 (4)	0.01437 (2)
Cl1	0.40606 (4)	0.15616 (2)	0.956246 (16)	0.02241 (6)
O1	0.29055 (11)	0.30392 (7)	0.83558 (5)	0.01747 (16)
O2	0.11079 (11)	0.20667 (7)	0.76526 (5)	0.01919 (17)
O3	-0.03497 (11)	0.56098 (7)	0.82164 (5)	0.01848 (16)
O4	0.73247 (14)	-0.13409 (9)	0.91070 (7)	0.0300 (2)
O5	0.65369 (15)	-0.16195 (9)	0.80196 (7)	0.0315 (2)
N1	0.65602 (14)	-0.11287 (9)	0.85191 (7)	0.0221 (2)
C1	-0.01601 (14)	0.35355 (9)	0.86993 (6)	0.01578 (19)
C2	0.05009 (15)	0.30813 (10)	0.93321 (6)	0.0186 (2)
H2A	0.1583	0.3075	0.9535	0.022*
C3	-0.04454 (18)	0.26366 (11)	0.96633 (7)	0.0228 (2)
H3A	0.0006	0.2345	1.0088	0.027*

supplementary materials

C4	-0.20606 (18)	0.26288 (11)	0.93602 (8)	0.0256 (3)
H4A	-0.2691	0.2331	0.9581	0.031*
C5	-0.27347 (17)	0.30654 (12)	0.87268 (8)	0.0262 (3)
H5A	-0.3815	0.3053	0.8521	0.031*
C6	-0.17904 (15)	0.35222 (11)	0.84008 (7)	0.0220 (2)
H6A	-0.2248	0.3822	0.7980	0.026*
C7	0.02070 (15)	0.43698 (9)	0.71033 (6)	0.0180 (2)
C8	-0.09430 (16)	0.37151 (10)	0.67264 (7)	0.0212 (2)
H8A	-0.1250	0.3196	0.6949	0.025*
C9	-0.16407 (19)	0.38189 (13)	0.60273 (7)	0.0279 (3)
H9A	-0.2413	0.3379	0.5786	0.033*
C10	-0.1169 (2)	0.45913 (14)	0.56922 (8)	0.0311 (3)
H10A	-0.1608	0.4660	0.5223	0.037*
C11	-0.0041 (2)	0.52566 (12)	0.60623 (8)	0.0294 (3)
H11A	0.0261	0.5777	0.5840	0.035*
C12	0.06386 (17)	0.51509 (10)	0.67604 (7)	0.0229 (2)
H12A	0.1388	0.5603	0.7003	0.027*
C13	0.31789 (14)	0.51920 (9)	0.86282 (7)	0.0173 (2)
C14	0.30934 (16)	0.61928 (10)	0.84459 (8)	0.0217 (2)
H14A	0.2159	0.6449	0.8156	0.026*
C15	0.43893 (17)	0.68101 (11)	0.86929 (8)	0.0252 (3)
H15A	0.4316	0.7472	0.8566	0.030*
C16	0.57927 (17)	0.64392 (11)	0.91288 (8)	0.0250 (3)
H16A	0.6659	0.6850	0.9293	0.030*
C17	0.58899 (17)	0.54502 (12)	0.93165 (8)	0.0249 (3)
H17A	0.6824	0.5199	0.9610	0.030*
C18	0.45934 (15)	0.48302 (10)	0.90679 (7)	0.0206 (2)
H18A	0.4673	0.4169	0.9197	0.025*
C19	0.24398 (14)	0.22178 (9)	0.80545 (6)	0.01492 (18)
C20	0.36213 (13)	0.13888 (9)	0.82013 (6)	0.01443 (18)
C21	0.39401 (15)	0.09388 (10)	0.76536 (6)	0.0179 (2)
H21A	0.3483	0.1191	0.7217	0.021*
C22	0.49241 (15)	0.01247 (10)	0.77476 (7)	0.0191 (2)
H22A	0.5136	-0.0170	0.7382	0.023*
C23	0.55811 (14)	-0.02348 (9)	0.84060 (7)	0.0172 (2)
C24	0.53294 (15)	0.02005 (9)	0.89647 (7)	0.0176 (2)
H24A	0.5799	-0.0050	0.9401	0.021*
C25	0.43558 (14)	0.10218 (9)	0.88556 (6)	0.01563 (19)
C26	-0.02762 (18)	0.60801 (11)	0.88443 (7)	0.0240 (2)
H26A	-0.0895	0.6672	0.8750	0.036*
H26B	0.0791	0.6244	0.9092	0.036*
H26D	-0.0675	0.5639	0.9111	0.036*
H1O3	-0.061 (3)	0.600 (2)	0.7921 (13)	0.042 (7)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01494 (4)	0.01250 (4)	0.01648 (4)	-0.00049 (2)	0.00621 (3)	0.00090 (3)

C11	0.03009 (15)	0.02303 (13)	0.01545 (12)	0.00816 (11)	0.00921 (10)	0.00142 (10)
O1	0.0181 (4)	0.0137 (4)	0.0201 (4)	0.0010 (3)	0.0055 (3)	-0.0007 (3)
O2	0.0163 (4)	0.0168 (4)	0.0221 (4)	0.0006 (3)	0.0028 (3)	0.0003 (3)
O3	0.0205 (4)	0.0156 (4)	0.0193 (4)	0.0028 (3)	0.0063 (3)	-0.0005 (3)
O4	0.0276 (5)	0.0227 (5)	0.0402 (6)	0.0081 (4)	0.0116 (5)	0.0084 (4)
O5	0.0357 (6)	0.0223 (5)	0.0446 (7)	0.0030 (4)	0.0243 (5)	-0.0055 (5)
N1	0.0202 (5)	0.0152 (4)	0.0354 (6)	0.0010 (4)	0.0152 (4)	0.0017 (4)
C1	0.0150 (4)	0.0148 (5)	0.0181 (5)	-0.0006 (4)	0.0063 (4)	0.0003 (4)
C2	0.0192 (5)	0.0196 (5)	0.0173 (5)	0.0004 (4)	0.0062 (4)	0.0006 (4)
C3	0.0295 (6)	0.0213 (6)	0.0208 (5)	0.0000 (5)	0.0124 (5)	0.0021 (4)
C4	0.0281 (6)	0.0227 (6)	0.0327 (7)	-0.0043 (5)	0.0191 (6)	0.0002 (5)
C5	0.0179 (5)	0.0258 (6)	0.0369 (7)	-0.0027 (5)	0.0117 (5)	0.0017 (6)
C6	0.0164 (5)	0.0232 (6)	0.0254 (6)	-0.0007 (4)	0.0051 (4)	0.0045 (5)
C7	0.0198 (5)	0.0161 (5)	0.0184 (5)	0.0027 (4)	0.0068 (4)	0.0011 (4)
C8	0.0223 (5)	0.0190 (5)	0.0198 (5)	-0.0003 (4)	0.0030 (4)	0.0000 (4)
C9	0.0295 (7)	0.0317 (7)	0.0188 (6)	0.0060 (6)	0.0028 (5)	-0.0015 (5)
C10	0.0347 (8)	0.0397 (8)	0.0186 (6)	0.0145 (7)	0.0080 (5)	0.0054 (6)
C11	0.0379 (8)	0.0268 (7)	0.0282 (7)	0.0095 (6)	0.0173 (6)	0.0111 (5)
C12	0.0274 (6)	0.0193 (5)	0.0246 (6)	0.0022 (5)	0.0121 (5)	0.0034 (5)
C13	0.0170 (5)	0.0158 (5)	0.0211 (5)	-0.0021 (4)	0.0088 (4)	-0.0014 (4)
C14	0.0191 (5)	0.0151 (5)	0.0325 (7)	-0.0016 (4)	0.0104 (5)	-0.0015 (5)
C15	0.0243 (6)	0.0172 (5)	0.0371 (7)	-0.0055 (5)	0.0140 (5)	-0.0038 (5)
C16	0.0229 (6)	0.0256 (6)	0.0282 (6)	-0.0084 (5)	0.0108 (5)	-0.0061 (5)
C17	0.0201 (6)	0.0289 (7)	0.0240 (6)	-0.0043 (5)	0.0049 (5)	-0.0013 (5)
C18	0.0199 (5)	0.0206 (5)	0.0215 (5)	-0.0023 (4)	0.0070 (4)	0.0002 (4)
C19	0.0160 (4)	0.0140 (4)	0.0156 (4)	0.0007 (4)	0.0062 (4)	0.0025 (4)
C20	0.0142 (4)	0.0138 (4)	0.0159 (4)	-0.0004 (4)	0.0057 (4)	0.0007 (4)
C21	0.0168 (5)	0.0217 (5)	0.0156 (5)	0.0012 (4)	0.0058 (4)	-0.0006 (4)
C22	0.0178 (5)	0.0212 (5)	0.0205 (5)	0.0002 (4)	0.0094 (4)	-0.0033 (4)
C23	0.0162 (5)	0.0133 (4)	0.0244 (5)	0.0009 (4)	0.0096 (4)	0.0006 (4)
C24	0.0189 (5)	0.0156 (5)	0.0193 (5)	0.0026 (4)	0.0077 (4)	0.0033 (4)
C25	0.0176 (5)	0.0147 (4)	0.0155 (5)	0.0012 (4)	0.0067 (4)	0.0006 (4)
C26	0.0268 (6)	0.0243 (6)	0.0232 (6)	0.0026 (5)	0.0112 (5)	-0.0036 (5)

Geometric parameters (Å, °)

Sn1—C1	2.1218 (12)	C10—C11	1.389 (3)
Sn1—C13	2.1339 (12)	C10—H10A	0.9300
Sn1—C7	2.1346 (13)	C11—C12	1.386 (2)
Sn1—O1	2.1737 (9)	C11—H11A	0.9300
Sn1—O3	2.3477 (9)	C12—H12A	0.9300
C11—C25	1.7344 (12)	C13—C18	1.3958 (18)
O1—C19	1.2772 (15)	C13—C14	1.4008 (18)
O2—C19	1.2385 (15)	C14—C15	1.3929 (19)
O3—C26	1.4320 (17)	C14—H14A	0.9300
O3—H103	0.78 (3)	C15—C16	1.390 (2)
O4—N1	1.2256 (18)	C15—H15A	0.9300
O5—N1	1.2252 (17)	C16—C17	1.388 (2)
N1—C23	1.4709 (17)	C16—H16A	0.9300

supplementary materials

C1—C2	1.3965 (17)	C17—C18	1.3959 (19)
C1—C6	1.4001 (17)	C17—H17A	0.9300
C2—C3	1.3944 (19)	C18—H18A	0.9300
C2—H2A	0.9300	C19—C20	1.5091 (16)
C3—C4	1.389 (2)	C20—C25	1.3951 (16)
C3—H3A	0.9300	C20—C21	1.3989 (17)
C4—C5	1.389 (2)	C21—C22	1.3883 (18)
C4—H4A	0.9300	C21—H21A	0.9300
C5—C6	1.393 (2)	C22—C23	1.3892 (19)
C5—H5A	0.9300	C22—H22A	0.9300
C6—H6A	0.9300	C23—C24	1.3831 (18)
C7—C8	1.3957 (18)	C24—C25	1.3888 (17)
C7—C12	1.3978 (19)	C24—H24A	0.9300
C8—C9	1.3889 (19)	C26—H26A	0.9600
C8—H8A	0.9300	C26—H26B	0.9600
C9—C10	1.396 (3)	C26—H26D	0.9600
C9—H9A	0.9300		
C1—Sn1—C13	126.30 (5)	C10—C11—H11A	119.7
C1—Sn1—C7	116.22 (5)	C11—C12—C7	120.54 (14)
C13—Sn1—C7	114.92 (5)	C11—C12—H12A	119.7
C1—Sn1—O1	94.17 (4)	C7—C12—H12A	119.7
C13—Sn1—O1	86.84 (4)	C18—C13—C14	118.29 (12)
C7—Sn1—O1	105.92 (4)	C18—C13—Sn1	121.67 (9)
C1—Sn1—O3	82.95 (4)	C14—C13—Sn1	119.91 (9)
C13—Sn1—O3	86.40 (4)	C15—C14—C13	120.90 (13)
C7—Sn1—O3	84.75 (4)	C15—C14—H14A	119.6
O1—Sn1—O3	169.05 (3)	C13—C14—H14A	119.6
C19—O1—Sn1	117.97 (8)	C16—C15—C14	120.21 (14)
C26—O3—Sn1	121.80 (8)	C16—C15—H15A	119.9
C26—O3—H103	109.1 (19)	C14—C15—H15A	119.9
Sn1—O3—H103	122.4 (19)	C17—C16—C15	119.46 (13)
O5—N1—O4	124.42 (13)	C17—C16—H16A	120.3
O5—N1—C23	117.74 (12)	C15—C16—H16A	120.3
O4—N1—C23	117.83 (12)	C16—C17—C18	120.39 (14)
C2—C1—C6	118.57 (12)	C16—C17—H17A	119.8
C2—C1—Sn1	122.08 (9)	C18—C17—H17A	119.8
C6—C1—Sn1	119.35 (9)	C13—C18—C17	120.76 (13)
C3—C2—C1	120.64 (12)	C13—C18—H18A	119.6
C3—C2—H2A	119.7	C17—C18—H18A	119.6
C1—C2—H2A	119.7	O2—C19—O1	124.55 (11)
C4—C3—C2	120.09 (13)	O2—C19—C20	118.82 (11)
C4—C3—H3A	120.0	O1—C19—C20	116.63 (10)
C2—C3—H3A	120.0	C25—C20—C21	118.55 (11)
C3—C4—C5	119.97 (13)	C25—C20—C19	122.89 (10)
C3—C4—H4A	120.0	C21—C20—C19	118.50 (10)
C5—C4—H4A	120.0	C22—C21—C20	121.44 (11)
C4—C5—C6	119.91 (13)	C22—C21—H21A	119.3
C4—C5—H5A	120.0	C20—C21—H21A	119.3
C6—C5—H5A	120.0	C21—C22—C23	117.76 (11)

C5—C6—C1	120.81 (13)	C21—C22—H22A	121.1
C5—C6—H6A	119.6	C23—C22—H22A	121.1
C1—C6—H6A	119.6	C24—C23—C22	122.79 (11)
C8—C7—C12	118.27 (12)	C24—C23—N1	118.00 (12)
C8—C7—Sn1	121.79 (10)	C22—C23—N1	119.19 (12)
C12—C7—Sn1	119.88 (10)	C23—C24—C25	118.10 (11)
C9—C8—C7	121.64 (14)	C23—C24—H24A	120.9
C9—C8—H8A	119.2	C25—C24—H24A	120.9
C7—C8—H8A	119.2	C24—C25—C20	121.29 (11)
C8—C9—C10	119.19 (15)	C24—C25—Cl1	117.47 (9)
C8—C9—H9A	120.4	C20—C25—Cl1	121.23 (9)
C10—C9—H9A	120.4	O3—C26—H26A	109.5
C11—C10—C9	119.78 (14)	O3—C26—H26B	109.5
C11—C10—H10A	120.1	H26A—C26—H26B	109.5
C9—C10—H10A	120.1	O3—C26—H26D	109.5
C12—C11—C10	120.55 (14)	H26A—C26—H26D	109.5
C12—C11—H11A	119.7	H26B—C26—H26D	109.5
C1—Sn1—O1—C19	67.75 (9)	C1—Sn1—C13—C18	70.01 (12)
C13—Sn1—O1—C19	-166.06 (9)	C7—Sn1—C13—C18	-128.94 (11)
C7—Sn1—O1—C19	-51.03 (10)	O1—Sn1—C13—C18	-22.84 (11)
O3—Sn1—O1—C19	142.03 (17)	O3—Sn1—C13—C18	148.55 (11)
C1—Sn1—O3—C26	66.69 (10)	C1—Sn1—C13—C14	-114.27 (11)
C13—Sn1—O3—C26	-60.57 (10)	C7—Sn1—C13—C14	46.78 (12)
C7—Sn1—O3—C26	-176.03 (10)	O1—Sn1—C13—C14	152.88 (11)
O1—Sn1—O3—C26	-8.6 (2)	O3—Sn1—C13—C14	-35.73 (10)
C13—Sn1—C1—C2	-43.07 (12)	C18—C13—C14—C15	0.4 (2)
C7—Sn1—C1—C2	156.10 (10)	Sn1—C13—C14—C15	-175.42 (11)
O1—Sn1—C1—C2	46.07 (11)	C13—C14—C15—C16	-0.2 (2)
O3—Sn1—C1—C2	-123.32 (11)	C14—C15—C16—C17	-0.1 (2)
C13—Sn1—C1—C6	136.78 (10)	C15—C16—C17—C18	0.3 (2)
C7—Sn1—C1—C6	-24.06 (12)	C14—C13—C18—C17	-0.3 (2)
O1—Sn1—C1—C6	-134.09 (10)	Sn1—C13—C18—C17	175.52 (11)
O3—Sn1—C1—C6	56.53 (10)	C16—C17—C18—C13	-0.1 (2)
C6—C1—C2—C3	-0.89 (19)	Sn1—O1—C19—O2	2.35 (16)
Sn1—C1—C2—C3	178.95 (10)	Sn1—O1—C19—C20	-178.31 (7)
C1—C2—C3—C4	1.0 (2)	O2—C19—C20—C25	-121.72 (13)
C2—C3—C4—C5	-0.1 (2)	O1—C19—C20—C25	58.90 (16)
C3—C4—C5—C6	-0.9 (2)	O2—C19—C20—C21	55.28 (16)
C4—C5—C6—C1	0.9 (2)	O1—C19—C20—C21	-124.10 (12)
C2—C1—C6—C5	-0.1 (2)	C25—C20—C21—C22	2.03 (19)
Sn1—C1—C6—C5	-179.91 (11)	C19—C20—C21—C22	-175.10 (11)
C1—Sn1—C7—C8	-25.33 (12)	C20—C21—C22—C23	0.30 (19)
C13—Sn1—C7—C8	171.64 (10)	C21—C22—C23—C24	-1.91 (19)
O1—Sn1—C7—C8	77.66 (11)	C21—C22—C23—N1	176.70 (11)
O3—Sn1—C7—C8	-104.81 (11)	O5—N1—C23—C24	166.13 (12)
C1—Sn1—C7—C12	151.78 (10)	O4—N1—C23—C24	-12.73 (18)
C13—Sn1—C7—C12	-11.26 (12)	O5—N1—C23—C22	-12.54 (18)
O1—Sn1—C7—C12	-105.24 (10)	O4—N1—C23—C22	168.60 (12)
O3—Sn1—C7—C12	72.30 (11)	C22—C23—C24—C25	1.09 (19)

supplementary materials

C12—C7—C8—C9	0.7 (2)	N1—C23—C24—C25	-177.53 (11)
Sn1—C7—C8—C9	177.85 (11)	C23—C24—C25—C20	1.37 (19)
C7—C8—C9—C10	0.7 (2)	C23—C24—C25—C11	-179.71 (10)
C8—C9—C10—C11	-1.5 (2)	C21—C20—C25—C24	-2.89 (18)
C9—C10—C11—C12	1.0 (2)	C19—C20—C25—C24	174.11 (11)
C10—C11—C12—C7	0.4 (2)	C21—C20—C25—C11	178.24 (9)
C8—C7—C12—C11	-1.2 (2)	C19—C20—C25—C11	-4.76 (17)
Sn1—C7—C12—C11	-178.43 (11)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H1O3 \cdots O2 ⁱ	0.79 (3)	1.83 (3)	2.6082 (14)	170 (3)
C16—H16A \cdots O4 ⁱⁱ	0.93	2.58	3.312 (2)	136

Symmetry codes: (i) $-x, y+1/2, -z+3/2$; (ii) $x, y+1, z$.

Fig. 1



Fig. 2

