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[3-(Dimethylamino)benzoato]triphenyltin(IV)

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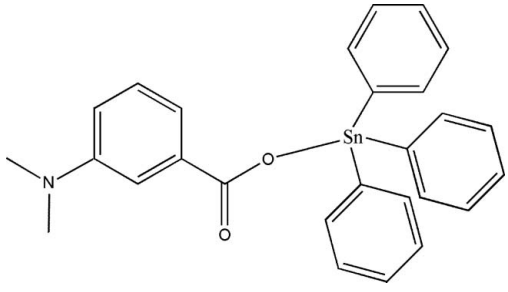
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.017; wR factor = 0.049; data-to-parameter ratio = 18.6.

In the title compound, $[Sn(C_6H_5)_3(C_9H_{10}NO_2)]$, the Sn atom is coordinated by three phenyl groups and a carboxylate anion in a distorted tetrahedral geometry. An intramolecular C—H···O interaction forms an S(7) ring motif. The dihedral angles between the benzoate group and the other three phenyl rings are 76.94 (8), 66.82 (8) and 42.34 (9)°. The crystal structure is further stabilized by intermolecular C—H···π interactions.

Related literature

For hydrogen-bond motifs, see Bernstein *et al.* (1995). For values of bond lengths, see Allen *et al.* (1987). For related literature on triorganotin(IV) complexes see, for example: Willem *et al.* (1997); Novelli *et al.* (1999); Gielen *et al.* (2000); Tian *et al.* (2005); Baul *et al.* (2001); Win *et al.* (2006, 2007*a*,*b*); Yeap & Teoh (2003).



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_9H_{10}NO_2)]$
M_r = 514.17
Triclinic, $P\overline{1}$
a = 9.1140 (2) Å
b = 10.0027 (2) Å
c = 14.5066 (4) Å
α = 100.925 (1)°
β = 103.106 (1)°
γ = 110.778 (1)°
V = 1150.13 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 100.0 (1) K
0.46 × 0.42 × 0.17 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.623, T_{max} = 0.830
18268 measured reflections
5259 independent reflections
5141 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.049
S = 1.08
5259 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—O1	2.0649 (11)	Sn1—C13	2.1260 (14)
Sn1—C1	2.1239 (15)	Sn1—C7	2.1290 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O2	0.93	2.43	3.126 (2)	132
C24—H24A···$Cg1^{i}$	0.93	2.88	3.6772 (19)	144
C26—H26B···$Cg2^{ii}$	0.96	2.74	3.672 (2)	164

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); 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, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2195).

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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.

Baul, T. S. B., Dhar, S., Pyke, S. M., Tiekink, E. R. T., Rivarola, E., Butcher, R. & Smith, F. E. (2001). *J. Organomet. Chem.* **633**, 7–17.

Bernstein, J., Davis, R. E., Shimoni, L. & Chamg, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Gielen, M., Biesemans, M., Vos, D. d. & Willem, R. (2000). *J. Inorg. Biochem.* **79**, 139–145.

Novelli, F., Recine, M., Sparatore, F. & Juliano, C. (1999). *Farmaco*, **54**, 237–241.

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

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Tian, L., Sun, Y., Li, H., Zheng, X., Cheng, Y., Liu, X. & Qian, B. (2005). *J. Inorg. Biochem.* **99**, 1646–1652.

Willem, R., Bunhdid, A., Mahieu, B., Ghys, L., Biesemans, M., Tiekink, E. R. T., Vos, D. d. & Gielen, M. (1997). *J. Organomet. Chem.* **531**, 151–158.

Win, Y. F., Guan, T. S., Ismail, N. L. & Yamin, B. M. (2006). *Acta Cryst.* E**62**, m3146–m3148.

Win, Y. F., Teoh, S.-G., Ng, S.-L., Fun, H.-K. & Ahmad, S. (2007*a*). *Acta Cryst.* E**63**, m2220–m2221.

Win, Y. F., Teoh, S. G., Teh, J. B. J., Fun, H.-K. & Zakaria, L. (2007*b*). *Acta Cryst.* E**63**, m323–m325.

Yeap, L.-L. & Teoh, S. G. (2003). *J. Coord. Chem.* **56**, 701–708.

supporting information

Acta Cryst. (2008). E**64**, m1530–m1531 [doi:10.1107/S1600536808036337]

[3-(Dimethylamino)benzoato]triphenyltin(IV)

Yip Foo Win, Siang Guan Teoh, Sie Tiong Ha, Reza Kia and Hoong-Kun Fun

S1. Comment

Triorganotin(IV) complexes are well known for their biological properties as well as industrial applications (Willem *et al.*, 1997; Novelli *et al.*, 1999; Gielen *et al.*, 2000; Tian *et al.*, 2005). Generally, triphenyltin(IV) carboxylate complexes are commonly found as monomeric structures with four-coordinated distorted tetrahedral or five-coordinated trigonal bipyramid geometries (Baul *et al.*, 2001; Yeap & Teoh, 2003; Win *et al.*, 2007*b*). In a recent study, the coordination geometry of (3,5-dinitrobenzoato)triphenyltin(IV) is found to be distorted tetrahedral due to the long range interaction of the carboxylate anion coordinated to the Sn moiety in an isobidentate fashion (Win *et al.*, 2006). In addition, triphenyltin(IV) carboxylates are also able to form polymeric structures (Tian *et al.*, 2005; Win *et al.*, 2007a). In the polymeric system, the carboxylate anions act as bridging bidentate ligands in the bonding to the neighbouring tin(IV) resulting in a polymeric structure with the tin atom exhibiting trigonal bipyramid geometry as shown in the complex, *catena*-poly[[triphenyltin(IV)–2,4-dinitrobenzoato] (Win *et al.*, 2007a). Based on the crystallographic structural study, the title complex [3-(dimethylamino)benzoato]triphenyltin(IV) has a monomeric four-coordinated distorted tetrahedral structure which is similar to that found for [4-(diethylamino)benzoato-*κ*O]triphenyltin(IV) (Win *et al.*, 2007*b*).

The bond lengths (Allen *et al.*, 1987) and angles in the molecule (I, Fig. 1, Table 1) are within normal ranges. The Sn atom is coordinated by the three phenyl groups and a carboxylate anion in a distorted tetrahedral geometry. An intramolecular hydrogen bond C—H···O forms a seven-membered ring, characterized as *S(7)* motif (Bernstein *et al.*, 1995). The dihedral angles between the phenyl-carboxylate group and the other three phenyl rings are 76.94 (8), 66.82 (8), and 42.34 (9)°, respectively. The crystal structure (Fig. 2), is further stabilized by intermolecular C—H···π (*x* 2) (Table 2) interactions.

S2. Experimental

The complex [3-(dimethylamino)benzoato]triphenyltin(IV) was obtained by heating under reflux a 1:1 molar mixture of triphenyltin(IV) hydroxide (1.10 g, 3 mmol) and 3-(dimethylamino)benzoic acid (0.50 g, 3 mmol) in acetonitrile (50 ml) for an hour. The clear brown solution was isolated by filtration and kept in a bottle. After eight days, brown crystals (1.01 g, 65.7% yield) were collected. Melting point: 413.2–414.5 K. Analysis found for $C_{27}H_{25}NO_2Sn$: C, 63.05; H, 4.91; N, 2.67; Sn, 23.00%. Calculated found for $C_{27}H_{25}NO_2Sn$: C, 63.07; H, 4.90; N, 2.72; Sn, 23.08%. FTIR as KBr disc (cm_{-1}): υ (C—H) aromatic 3065, 3051, 3026; υ (C—H) saturated 2989, 2908, 2810; υ $(COO)_{as}$ 1625, υ $(COO)_s$ 1322, υ (C—N) 1227, υ (Sn—O) 445. ^{1}H-NMR: δ: phenyl protons 7.42–7.49 (9*H*, m); 7.79–7.81 (6*H*, m); benzene 6.86–6.88 (1*H*, dd); 7.24–7.28 (1*H*, t); 7.51–7.53 (2*H*, d); N-(CH3)2 2.95 (6*H*, s) p.p.m.. ^{13}C-NMR: δ: phenyl carbons C_{ipso} 139.01 (648.9 Hz), C_{ortho} 137.36 (47.9 Hz), C_{meta} 129.31 (63.2 Hz), C_{para} 130.28; benzene 114.84, 117.18, 119.31, 129.57, 134.59, 150.85; N-$(CH_3)_2$ 41.04; COO 174.05 p.p.m.. ^{119}Sn-NMR: υ: -114.19 p.p.m..

S3. Refinement

All of the hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å for aromatic H and 0.96 Å for methyl H atoms. A rotating group model was used for the methyl groups.

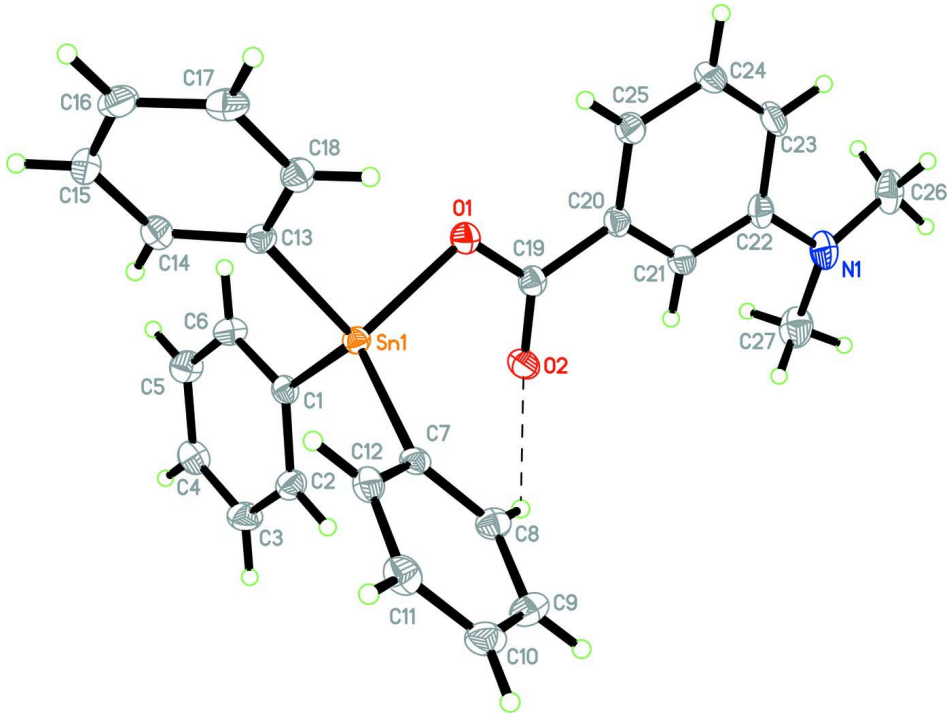

Figure 1

The molecular structure of the title compound with atom lables and the 50% probability ellipsoids for non-H atoms. Intramolecular hydrogen bonds is shown as dashed lines.

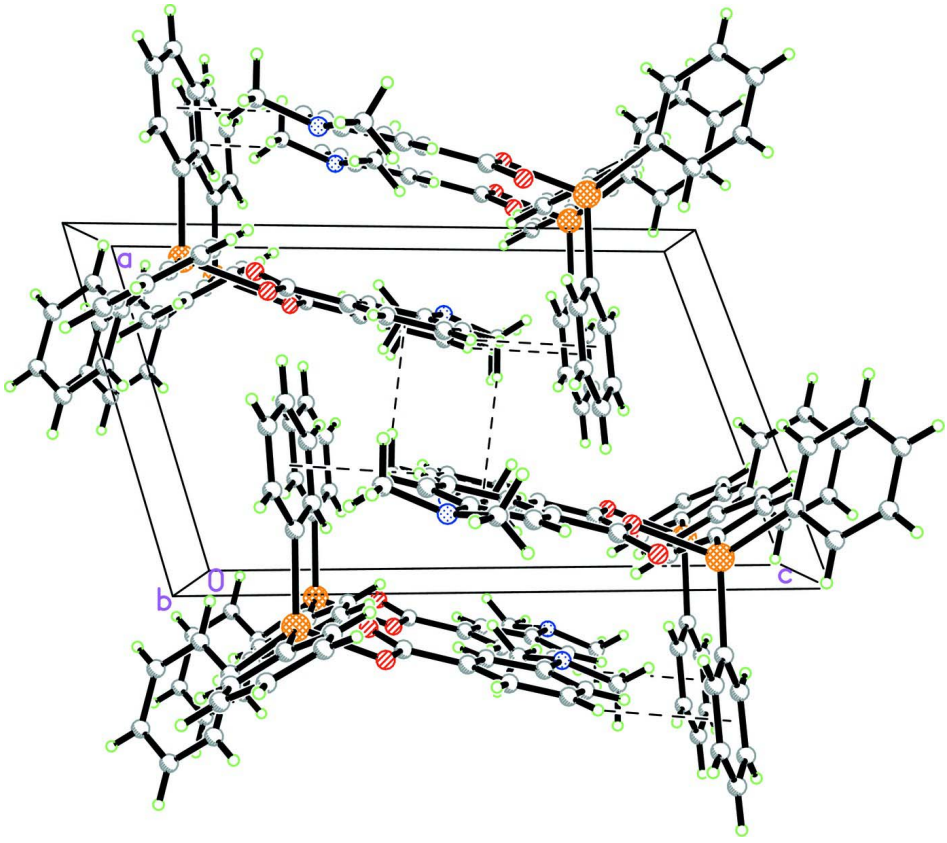

Figure 2

The crystal structure of (I), viewed down the *b*-axis. Intermolecular C—H···π interactions were shown as dashed lines.

[3-(Dimethylamino)benzoato]triphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_9H_{10}NO_2)]$
M_r = 514.17
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.1140 (2) Å
b = 10.0027 (2) Å
c = 14.5066 (4) Å
α = 100.925 (1)°
β = 103.106 (1)°
γ = 110.778 (1)°
V = 1150.13 (5) Å^3
Z = 2
$F(000)$ = 520
D_x = 1.485 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9986 reflections
θ = 2.5–31.2°
μ = 1.13 mm^{-1}
T = 100 K
Block, colourless
0.46 × 0.42 × 0.17 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.623, T_{max} = 0.830
18268 measured reflections
5259 independent reflections
5141 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −11→11
k = −12→12
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.049$
$S = 1.08$
5259 reflections
282 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.592P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Special details

Experimental. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.
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}
Sn1	0.091614 (11)	0.100499 (9)	0.838745 (6)	0.01429 (4)
O1	0.18084 (14)	0.11930 (12)	0.72088 (8)	0.0197 (2)
O2	0.11484 (14)	0.31350 (12)	0.73771 (8)	0.0204 (2)
N1	0.22892 (18)	0.51484 (16)	0.45101 (10)	0.0254 (3)
C1	0.22847 (18)	0.28442 (15)	0.96940 (10)	0.0159 (3)
C2	0.14887 (19)	0.36829 (17)	1.00604 (11)	0.0207 (3)
H2A	0.0400	0.3462	0.9710	0.025*
C3	0.2303 (2)	0.48439 (18)	1.09426 (12)	0.0244 (3)
H3A	0.1762	0.5399	1.1177	0.029*
C4	0.3920 (2)	0.51738 (17)	1.14722 (12)	0.0229 (3)
H4A	0.4465	0.5948	1.2064	0.028*
C5	0.4729 (2)	0.43461 (18)	1.11195 (12)	0.0232 (3)
H5A	0.5816	0.4570	1.1474	0.028*
C6	0.39153 (19)	0.31856 (17)	1.02389 (12)	0.0205 (3)
H6A	0.4459	0.2631	1.0010	0.025*
C7	−0.16663 (18)	0.04727 (16)	0.79258 (10)	0.0158 (3)
C8	−0.23183 (19)	0.14256 (16)	0.75791 (11)	0.0194 (3)
H8A	−0.1615	0.2315	0.7516	0.023*
C9	−0.4012 (2)	0.10510 (18)	0.73291 (12)	0.0233 (3)
H9A	−0.4435	0.1683	0.7089	0.028*
C10	−0.5073 (2)	−0.02620 (19)	0.74368 (12)	0.0240 (3)
H10A	−0.6201	−0.0501	0.7280	0.029*
C11	−0.4443 (2)	−0.12170 (18)	0.77797 (12)	0.0230 (3)
H11A	−0.5151	−0.2100	0.7849	0.028*

C12	−0.27509 (19)	−0.08543 (17)	0.80205 (11)	0.0188 (3)
H12A	−0.2338	−0.1501	0.8247	0.023*
C13	0.13625 (18)	−0.08981 (16)	0.85493 (11)	0.0164 (3)
C14	0.2177 (2)	−0.09087 (18)	0.94868 (12)	0.0215 (3)
H14A	0.2560	−0.0066	1.0028	0.026*
C15	0.2422 (2)	−0.21653 (19)	0.96204 (12)	0.0251 (3)
H15A	0.2965	−0.2160	1.0248	0.030*
C16	0.1856 (2)	−0.34238 (18)	0.88169 (13)	0.0245 (3)
H16A	0.1999	−0.4271	0.8907	0.029*
C17	0.1073 (2)	−0.34218 (17)	0.78765 (13)	0.0225 (3)
H17A	0.0713	−0.4260	0.7336	0.027*
C18	0.08268 (18)	−0.21649 (17)	0.77429 (11)	0.0193 (3)
H18A	0.0302	−0.2169	0.7112	0.023*
C19	0.16464 (18)	0.23129 (16)	0.69218 (11)	0.0168 (3)
C20	0.20934 (18)	0.25094 (16)	0.60128 (10)	0.0172 (3)
C21	0.20685 (18)	0.37521 (16)	0.57167 (11)	0.0184 (3)
H21A	0.1814	0.4443	0.6098	0.022*
C22	0.24224 (19)	0.39733 (17)	0.48506 (11)	0.0199 (3)
C23	0.2867 (2)	0.29256 (19)	0.43204 (11)	0.0239 (3)
H23A	0.3153	0.3064	0.3758	0.029*
C24	0.2888 (2)	0.16944 (19)	0.46203 (12)	0.0246 (3)
H24A	0.3171	0.1014	0.4251	0.030*
C25	0.24929 (19)	0.14608 (17)	0.54641 (11)	0.0207 (3)
H25A	0.2494	0.0627	0.5659	0.025*
C26	0.2998 (2)	0.5495 (2)	0.37333 (13)	0.0306 (4)
H26A	0.2477	0.4636	0.3157	0.046*
H26B	0.4166	0.5755	0.3964	0.046*
H26C	0.2817	0.6321	0.3568	0.046*
C27	0.2286 (2)	0.64104 (19)	0.52007 (14)	0.0318 (4)
H27A	0.1372	0.6063	0.5449	0.048*
H27B	0.2177	0.7127	0.4865	0.048*
H27C	0.3305	0.6873	0.5743	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01477 (6)	0.01395 (6)	0.01457 (6)	0.00679 (4)	0.00447 (4)	0.00385 (4)
O1	0.0237 (5)	0.0211 (5)	0.0189 (5)	0.0116 (4)	0.0093 (4)	0.0091 (4)
O2	0.0243 (6)	0.0207 (5)	0.0194 (5)	0.0105 (4)	0.0108 (4)	0.0065 (4)
N1	0.0309 (7)	0.0256 (7)	0.0197 (6)	0.0100 (6)	0.0072 (6)	0.0110 (5)
C1	0.0177 (7)	0.0146 (6)	0.0149 (6)	0.0058 (5)	0.0057 (5)	0.0047 (5)
C2	0.0187 (7)	0.0234 (7)	0.0200 (7)	0.0105 (6)	0.0043 (6)	0.0057 (6)
C3	0.0273 (8)	0.0245 (8)	0.0235 (8)	0.0143 (7)	0.0097 (7)	0.0029 (6)
C4	0.0250 (8)	0.0190 (7)	0.0189 (7)	0.0055 (6)	0.0057 (6)	0.0018 (6)
C5	0.0176 (7)	0.0235 (7)	0.0231 (8)	0.0060 (6)	0.0035 (6)	0.0042 (6)
C6	0.0180 (7)	0.0206 (7)	0.0231 (7)	0.0093 (6)	0.0067 (6)	0.0041 (6)
C7	0.0155 (6)	0.0180 (6)	0.0125 (6)	0.0076 (5)	0.0041 (5)	0.0005 (5)
C8	0.0193 (7)	0.0170 (6)	0.0205 (7)	0.0079 (6)	0.0059 (6)	0.0028 (5)

C9	0.0210 (7)	0.0223 (7)	0.0268 (8)	0.0122 (6)	0.0050 (6)	0.0045 (6)
C10	0.0162 (7)	0.0289 (8)	0.0228 (8)	0.0082 (6)	0.0055 (6)	0.0023 (6)
C11	0.0200 (7)	0.0239 (7)	0.0205 (7)	0.0044 (6)	0.0067 (6)	0.0054 (6)
C12	0.0203 (7)	0.0198 (7)	0.0149 (7)	0.0077 (6)	0.0045 (6)	0.0042 (5)
C13	0.0151 (6)	0.0169 (6)	0.0198 (7)	0.0076 (5)	0.0072 (5)	0.0072 (5)
C14	0.0257 (8)	0.0234 (7)	0.0180 (7)	0.0120 (6)	0.0084 (6)	0.0064 (6)
C15	0.0289 (8)	0.0341 (9)	0.0236 (8)	0.0196 (7)	0.0119 (7)	0.0163 (7)
C16	0.0256 (8)	0.0245 (8)	0.0366 (9)	0.0162 (6)	0.0178 (7)	0.0167 (7)
C17	0.0217 (7)	0.0175 (7)	0.0296 (8)	0.0088 (6)	0.0115 (6)	0.0047 (6)
C18	0.0175 (7)	0.0195 (7)	0.0192 (7)	0.0073 (6)	0.0045 (6)	0.0050 (6)
C19	0.0147 (6)	0.0174 (6)	0.0152 (6)	0.0048 (5)	0.0031 (5)	0.0041 (5)
C20	0.0161 (7)	0.0199 (7)	0.0135 (6)	0.0063 (5)	0.0035 (5)	0.0041 (5)
C21	0.0186 (7)	0.0191 (7)	0.0158 (7)	0.0075 (5)	0.0044 (5)	0.0038 (5)
C22	0.0183 (7)	0.0223 (7)	0.0146 (7)	0.0053 (6)	0.0022 (5)	0.0055 (6)
C23	0.0256 (8)	0.0325 (8)	0.0127 (7)	0.0114 (7)	0.0068 (6)	0.0056 (6)
C24	0.0280 (8)	0.0300 (8)	0.0156 (7)	0.0150 (7)	0.0065 (6)	0.0009 (6)
C25	0.0228 (7)	0.0211 (7)	0.0170 (7)	0.0101 (6)	0.0043 (6)	0.0035 (6)
C26	0.0266 (8)	0.0360 (9)	0.0241 (8)	0.0052 (7)	0.0054 (7)	0.0164 (7)
C27	0.0408 (10)	0.0243 (8)	0.0311 (9)	0.0139 (7)	0.0091 (8)	0.0125 (7)

Geometric parameters (Å, º)

Sn1—O1	2.0649 (11)	C12—H12A	0.9300
Sn1—C1	2.1239 (15)	C13—C18	1.397 (2)
Sn1—C13	2.1260 (14)	C13—C14	1.398 (2)
Sn1—C7	2.1290 (14)	C14—C15	1.393 (2)
O1—C19	1.3101 (17)	C14—H14A	0.9300
O2—C19	1.2303 (19)	C15—C16	1.385 (2)
N1—C22	1.391 (2)	C15—H15A	0.9300
N1—C27	1.457 (2)	C16—C17	1.389 (2)
N1—C26	1.458 (2)	C16—H16A	0.9300
C1—C2	1.397 (2)	C17—C18	1.393 (2)
C1—C6	1.398 (2)	C17—H17A	0.9300
C2—C3	1.390 (2)	C18—H18A	0.9300
C2—H2A	0.9300	C19—C20	1.493 (2)
C3—C4	1.384 (2)	C20—C21	1.396 (2)
C3—H3A	0.9300	C20—C25	1.397 (2)
C4—C5	1.391 (2)	C21—C22	1.404 (2)
C4—H4A	0.9300	C21—H21A	0.9300
C5—C6	1.388 (2)	C22—C23	1.411 (2)
C5—H5A	0.9300	C23—C24	1.386 (2)
C6—H6A	0.9300	C23—H23A	0.9300
C7—C12	1.399 (2)	C24—C25	1.390 (2)
C7—C8	1.401 (2)	C24—H24A	0.9300
C8—C9	1.393 (2)	C25—H25A	0.9300
C8—H8A	0.9300	C26—H26A	0.9600
C9—C10	1.389 (2)	C26—H26B	0.9600
C9—H9A	0.9300	C26—H26C	0.9600

C10—C11	1.389 (2)	C27—H27A	0.9600
C10—H10A	0.9300	C27—H27B	0.9600
C11—C12	1.394 (2)	C27—H27C	0.9600
C11—H11A	0.9300		

O1—Sn1—C1	114.69 (5)	C15—C14—C13	120.83 (15)
O1—Sn1—C13	95.46 (5)	C15—C14—H14A	119.6
C1—Sn1—C13	110.92 (6)	C13—C14—H14A	119.6
O1—Sn1—C7	109.89 (5)	C16—C15—C14	119.87 (15)
C1—Sn1—C7	113.28 (6)	C16—C15—H15A	120.1
C13—Sn1—C7	111.31 (5)	C14—C15—H15A	120.1
C19—O1—Sn1	109.13 (9)	C15—C16—C17	120.07 (14)
C22—N1—C27	118.52 (13)	C15—C16—H16A	120.0
C22—N1—C26	118.12 (15)	C17—C16—H16A	120.0
C27—N1—C26	115.85 (14)	C16—C17—C18	120.06 (15)
C2—C1—C6	118.61 (14)	C16—C17—H17A	120.0
C2—C1—Sn1	118.67 (11)	C18—C17—H17A	120.0
C6—C1—Sn1	122.57 (11)	C17—C18—C13	120.51 (14)
C3—C2—C1	120.82 (14)	C17—C18—H18A	119.7
C3—C2—H2A	119.6	C13—C18—H18A	119.7
C1—C2—H2A	119.6	O2—C19—O1	121.43 (13)
C4—C3—C2	119.94 (15)	O2—C19—C20	122.89 (13)
C4—C3—H3A	120.0	O1—C19—C20	115.68 (13)
C2—C3—H3A	120.0	C21—C20—C25	121.04 (14)
C3—C4—C5	119.97 (15)	C21—C20—C19	118.15 (13)
C3—C4—H4A	120.0	C25—C20—C19	120.80 (13)
C5—C4—H4A	120.0	C20—C21—C22	120.90 (14)
C6—C5—C4	120.12 (15)	C20—C21—H21A	119.6
C6—C5—H5A	119.9	C22—C21—H21A	119.6
C4—C5—H5A	119.9	N1—C22—C21	121.46 (15)
C5—C6—C1	120.54 (14)	N1—C22—C23	121.24 (14)
C5—C6—H6A	119.7	C21—C22—C23	117.27 (14)
C1—C6—H6A	119.7	C24—C23—C22	121.36 (14)
C12—C7—C8	118.59 (13)	C24—C23—H23A	119.3
C12—C7—Sn1	118.36 (10)	C22—C23—H23A	119.3
C8—C7—Sn1	122.97 (11)	C23—C24—C25	121.01 (15)
C9—C8—C7	120.51 (14)	C23—C24—H24A	119.5
C9—C8—H8A	119.7	C25—C24—H24A	119.5
C7—C8—H8A	119.7	C24—C25—C20	118.36 (14)
C10—C9—C8	120.31 (15)	C24—C25—H25A	120.8
C10—C9—H9A	119.8	C20—C25—H25A	120.8
C8—C9—H9A	119.8	N1—C26—H26A	109.5
C9—C10—C11	119.76 (15)	N1—C26—H26B	109.5
C9—C10—H10A	120.1	H26A—C26—H26B	109.5
C11—C10—H10A	120.1	N1—C26—H26C	109.5
C10—C11—C12	120.11 (15)	H26A—C26—H26C	109.5
C10—C11—H11A	119.9	H26B—C26—H26C	109.5
C12—C11—H11A	119.9	N1—C27—H27A	109.5

C11—C12—C7	120.71 (14)	N1—C27—H27B	109.5
C11—C12—H12A	119.6	H27A—C27—H27B	109.5
C7—C12—H12A	119.6	N1—C27—H27C	109.5
C18—C13—C14	118.64 (13)	H27A—C27—H27C	109.5
C18—C13—Sn1	121.68 (11)	H27B—C27—H27C	109.5
C14—C13—Sn1	119.66 (11)		

C1—Sn1—O1—C19	−65.43 (10)	C7—Sn1—C13—C18	63.64 (13)
C13—Sn1—O1—C19	178.55 (10)	O1—Sn1—C13—C14	131.33 (12)
C7—Sn1—O1—C19	63.54 (10)	C1—Sn1—C13—C14	12.27 (13)
O1—Sn1—C1—C2	118.11 (11)	C7—Sn1—C13—C14	−114.83 (12)
C13—Sn1—C1—C2	−135.17 (11)	C18—C13—C14—C15	−1.3 (2)
C7—Sn1—C1—C2	−9.16 (13)	Sn1—C13—C14—C15	177.23 (12)
O1—Sn1—C1—C6	−66.39 (13)	C13—C14—C15—C16	0.1 (2)
C13—Sn1—C1—C6	40.33 (13)	C14—C15—C16—C17	1.2 (2)
C7—Sn1—C1—C6	166.35 (11)	C15—C16—C17—C18	−1.3 (2)
C6—C1—C2—C3	0.7 (2)	C16—C17—C18—C13	0.0 (2)
Sn1—C1—C2—C3	176.37 (12)	C14—C13—C18—C17	1.3 (2)
C1—C2—C3—C4	−0.4 (2)	Sn1—C13—C18—C17	−177.23 (11)
C2—C3—C4—C5	0.2 (2)	Sn1—O1—C19—O2	5.06 (17)
C3—C4—C5—C6	−0.2 (2)	Sn1—O1—C19—C20	−174.58 (10)
C4—C5—C6—C1	0.5 (2)	O2—C19—C20—C21	5.3 (2)
C2—C1—C6—C5	−0.7 (2)	O1—C19—C20—C21	−175.11 (13)
Sn1—C1—C6—C5	−176.25 (11)	O2—C19—C20—C25	−173.49 (14)
O1—Sn1—C7—C12	120.58 (11)	O1—C19—C20—C25	6.1 (2)
C1—Sn1—C7—C12	−109.69 (11)	C25—C20—C21—C22	0.9 (2)
C13—Sn1—C7—C12	16.12 (13)	C19—C20—C21—C22	−177.86 (13)
O1—Sn1—C7—C8	−62.74 (13)	C27—N1—C22—C21	18.9 (2)
C1—Sn1—C7—C8	67.00 (13)	C26—N1—C22—C21	167.49 (15)
C13—Sn1—C7—C8	−167.20 (12)	C27—N1—C22—C23	−163.14 (16)
C12—C7—C8—C9	−0.4 (2)	C26—N1—C22—C23	−14.6 (2)
Sn1—C7—C8—C9	−177.08 (12)	C20—C21—C22—N1	175.44 (14)
C7—C8—C9—C10	1.1 (2)	C20—C21—C22—C23	−2.5 (2)
C8—C9—C10—C11	−1.1 (2)	N1—C22—C23—C24	−175.42 (15)
C9—C10—C11—C12	0.4 (2)	C21—C22—C23—C24	2.6 (2)
C10—C11—C12—C7	0.3 (2)	C22—C23—C24—C25	−0.9 (3)
C8—C7—C12—C11	−0.3 (2)	C23—C24—C25—C20	−0.8 (2)
Sn1—C7—C12—C11	176.53 (11)	C21—C20—C25—C24	0.9 (2)
O1—Sn1—C13—C18	−50.20 (12)	C19—C20—C25—C24	179.56 (14)
C1—Sn1—C13—C18	−169.26 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···O2	0.93	2.43	3.126 (2)	132

C24—H24*A*···*Cg*1^{i}	0.93	2.88	3.6772 (19)	144
C26—H26*B*···*Cg*2^{ii}	0.96	2.74	3.672 (2)	164

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