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catena-Poly[[triphenyltin(IV)]-μ-2,4-dinitrobenzoato]

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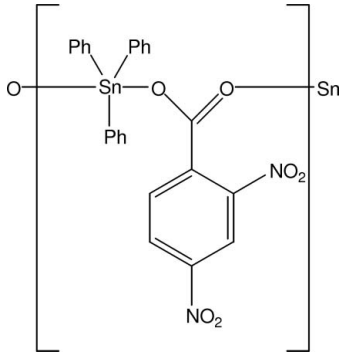
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.120; data-to-parameter ratio = 33.3.

In the title compound, $[Sn(C_{25}H_{18}N_2O_6)]_n$, the Sn atom shows a trigonal bipyramidal coordination with equatorial phenyl groups and axial carboxylates linking the metal atoms into a polymeric chain. The nitro groups are slightly twisted away from the attached aromatic ring. In the crystal structure, the chains are linked by intermolecular C—H···O interactions, forming columns along the b axis. In addition, the crystal structure is further stabilized by intermolecular π–π interactions, with centroid-to-centroid distance of 3.5538 (15) Å.

Related literature

For literature on hydrogen-bond motifs, see Bernstein *et al.* (1995). For data on bond lengths, see Allen *et al.* (1987). For related literature, see: Baul *et al.* (2001); Gielen *et al.* (2000); Novelli *et al.* (1999); Willem *et al.* (1997); Win *et al.* (2006); Win *et al.* (2007); Yeap & Teoh (2003).



Experimental

Crystal data

$[Sn(C_{25}H_{18}N_2O_6)]$
M_r = 561.10
Monoclinic, $P2_1/c$
a = 6.5835 (1) Å
b = 11.8399 (2) Å
c = 29.0173 (4) Å
β = 97.317 (1)°
V = 2243.42 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 100.0 (1) K
0.27 × 0.14 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan *SADABS* (Bruker, 2005)
T_{min} = 0.813, T_{max} = 0.887
45670 measured reflections
10230 independent reflections
8104 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.120
S = 1.10
10230 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C7	2.128 (2)	Sn1—O2^{i}	2.2370 (18)
Sn1—C1	2.130 (2)	Sn1—O1	2.2517 (17)
Sn1—C13	2.136 (2)		
C7—Sn1—C1	115.46 (9)	C13—Sn1—O2^{i}	87.22 (8)
C7—Sn1—C13	124.90 (9)	C7—Sn1—O1	87.89 (9)
C1—Sn1—C13	119.61 (9)	C1—Sn1—O1	93.78 (8)
C7—Sn1—O2^{i}	89.85 (9)	C13—Sn1—O1	86.75 (8)
C1—Sn1—O2^{i}	95.25 (8)	O2^{i}—Sn1—O1	170.79 (7)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O1	0.93	2.37	2.977 (3)	123
C18—H18A···O1	0.93	2.39	2.984 (3)	121
C12—H12A···O2^{i}	0.93	2.40	3.026 (3)	124
C14—H14A···O2^{i}	0.93	2.52	3.028 (3)	115
C17—H17A···O6^{ii}	0.93	2.47	3.331 (4)	153
C21—H21A···O5^{iii}	0.93	2.40	3.279 (3)	158

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); 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: BT2448).

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supplementary materials

Acta Cryst. (2007). E**63**, m2220-m2221 [**doi:10.1107/S1600536807035556**]

catena-Poly[[triphenyltin(IV)]-μ-2,4-dinitrobenzoato]

Y. F. Win, S.-G. Teoh, S.-L. Ng, H.-K. Fun and S. Ahmad

Comment

Besides their significant industrial applications (Willem *et al.*, 1997; Novelli *et al.*, 1999; Gielen *et al.*, 2000), organotin (IV) complexes are reported to exhibit antimicrobial and antitumour properties. Generally triphenyltin(IV) carboxylate complexes exist as monomeric structures with four-coordinate distorted tetrahedal or five-coordinate trigonal bypyramid geometries (Baul *et al.*, 2001; Yeap & Teoh, 2003; Win *et al.*, 2006). Recently, (3,5-dintrobenzoato)triphenyltin(IV) is reported to existed as a monomeric structure with four-coordinate distorted tetrahedral geometry (Win *et al.*, 2006). Both the nitro groups are substituted at *ortho* and *para* positions of the benzene rings in (2,4-dinitrobenzoato)triphenyl(IV) complex whereas the dinitro groups occupy the *meta* position in (3,5-dinitrobenzoato)triphenyltin(IV) complex. In the crystal structure, the title molecules form polymeric chains along the *a* axis. As such, the complex obtained in this study exist as a polymeric structure with a five-coordinate trigonal bypyramid geometry (Scheme). The Sn coordination is a distorted trigonal bipyramid (scheme and Table 1). Bond lengths and angles in (I) (Figure 1) have normal values (Allen *et al.*, 1987) and agree well with those found in related structures (Win *et al.*, 2007). The nitro groups at C23 and C25 are slightly twisted away from attached benzene rings with torsion angle O3—N1—C25—C20 = −14.2 (3)°, and O5—N2—C23—C22 = −16.7 (4)°, respectively.

The intramolecular C8—H8A···O1 and C18—H18A···O1 interactions (Table 1 and figure 1) generate S(5) ring motifs (Bernstein *et al.*, 1995). In the crystal structure, the molecules linked by intermolecular C17—H17A···O6, C21—H21A···O5, C12—H12A···O2 and C14—H14A···O2 interactions to form columns along the *b* axis (Figure 2). In addition, the crystal packing is further stabilized by the weak intermolecular π-π interactions involving the C1—C6 ring (centroid *Cg*1) and the C20—C25 (centroid *Cg*2) benzene rings with a $Cg1\cdots Cg2^{iv}$ distance of 3.5538 (15)Å [symmetry code: iv (1 + *x*, *y*, *z*)].

Experimental

The complex (2,4-dinitrobenzoato)diphenyltin(IV) was obtained by heating under reflux a 1:1 molar mixture of triphenyltin(IV) hydroxide (1.10 g, 3 mmole) and 2,4-dinitrobenzoic acid (0.64 g, 3 mmole) in ethanol (50 ml) for two hours. A clear yellowish solution was isolated by filtration and kept in a bottle. After two weeks, some yellowish precipitate (1.38 g, 82.3% yield) were obtained which are then recrystallized. Melting point: 160.4 − 161.2°C. Analysis found for $C_{25}H_{18}N_2O_6Sn$: C, 53.31; H, 3.00; N, 4.91; Sn. 21.03%; calculated for $C_{25}H_{18}N_2O_6Sn$: C, 53.51; H, 3.23; N, 5.00; Sn, 21.15%. FTIR as KBr disc (cm^{-1}): v(C—H) aromatic 3069, 3051, 3023; $v(COO)_{as}$ 1599, $v(COO)_s$ 1345, $v(NO_2)$ 1541, v(Sn—O) 453. ^{1}H-NMR: δ: phenyl protons 7.47 − 7.50 (9*H*, m); 7.75 − 7.78 (6*H*, m); benzene 7.90 − 7.92 (1*H*, d, J = 8.4 Hz); 8.35 − 8.38 (1*H*, dd, J = 8.4 Hz); 8.60 − 8.61 (1*H*, d, 2.1 Hz)p.p.m.. ^{13}C-NMR: δ:phenyl carbons C_{ipso} 137.68 (655.6 Hz), C_{ortho} 137.27 (48.9 Hz), C_{meta} 129,66 (65.1 Hz), C_{para} 131.17 (13.1 Hz); benzene 119.58, 127.26, 132.21, 134.58, 148,73, 148.97; COO 168.56 p.p.m.. ^{119}Sn-NMR: δ: −81.04 p.p.m..

Refinement

The H atoms were positional geometrically and treated as riding, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

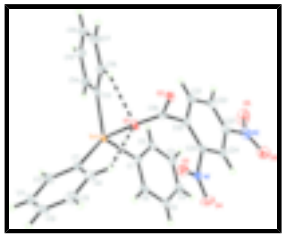

Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering. The dashed lines indicate intramolecular hydrogen bonds.

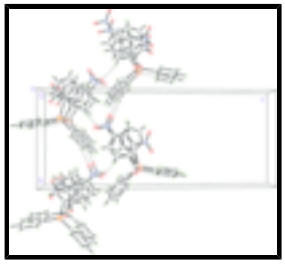

Fig. 2. The crystal packing of (I), viewed down the *a* axis. The intermolecular C—H···O hydrogen bonds are shown as dashed lines.

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Crystal data

$[Sn(C_{25}H_{18}N_2O_6)]$	F_{000} = 1120
M_r = 561.10	D_x = 1.661 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5968 reflections
a = 6.5835 (1) Å	θ = 1.4–35.6º
b = 11.8399 (2) Å	μ = 1.18 mm^{-1}
c = 29.0173 (4) Å	T = 100.0 (1) K
β = 97.317 (1)º	Block, colourless
V = 2243.42 (6) Å^3	0.27 × 0.14 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	10230 independent reflections
Radiation source: fine-focus sealed tube	8104 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 35.6º
T = 100.0(1) K	θ_{min} = 1.4º
ω scans	h = −10→9

Absorption correction: multi-scan SADABS (Bruker, 2005)

T_{min} = 0.813, T_{max} = 0.887

45670 measured reflections

k = −19→18

l = −47→47

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.038

$wR(F^2)$ = 0.120

S = 1.10

10230 reflections

307 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 2.2536P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.77 e Å^{-3}

$\Delta\rho_{min}$ = −0.87 e Å^{-3}

Extinction correction: none

Special details

Experimental. The 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	0.87124 (2)	0.294273 (13)	0.087817 (5)	0.01171 (5)
O1	0.5266 (3)	0.29990 (15)	0.07927 (7)	0.0159 (3)
O2	0.2108 (3)	0.31893 (15)	0.09542 (7)	0.0163 (3)
O3	0.2851 (3)	0.11530 (17)	0.03396 (6)	0.0215 (4)
O4	0.3619 (4)	−0.06212 (18)	0.04299 (7)	0.0272 (4)
O5	0.5299 (4)	−0.1099 (2)	0.25504 (9)	0.0421 (6)
O6	0.3845 (4)	−0.21551 (18)	0.19930 (9)	0.0334 (5)
N1	0.3405 (3)	0.03299 (19)	0.05774 (7)	0.0160 (4)
N2	0.4504 (4)	−0.1246 (2)	0.21479 (9)	0.0243 (5)
C1	0.8850 (4)	0.1206 (2)	0.10719 (8)	0.0140 (4)
C2	0.9165 (4)	0.0846 (2)	0.15348 (8)	0.0147 (4)
H2A	0.9314	0.1375	0.1773	0.018*
C3	0.9257 (4)	−0.0307 (2)	0.16399 (9)	0.0182 (4)

H3A	0.9486	−0.0540	0.1948	0.022*
C4	0.9008 (4)	−0.1108 (2)	0.12863 (10)	0.0205 (5)
H4A	0.9063	−0.1874	0.1358	0.025*
C5	0.8678 (4)	−0.0763 (2)	0.08267 (9)	0.0185 (5)
H5A	0.8503	−0.1297	0.0590	0.022*
C6	0.8607 (4)	0.0389 (2)	0.07174 (9)	0.0164 (4)
H6A	0.8397	0.0616	0.0408	0.020*
C7	0.8551 (4)	0.3266 (2)	0.01530 (8)	0.0161 (4)
C8	0.6708 (4)	0.3126 (2)	−0.01376 (9)	0.0200 (5)
H8A	0.5534	0.2914	−0.0012	0.024*
C9	0.6616 (5)	0.3300 (3)	−0.06136 (10)	0.0280 (6)
H9A	0.5379	0.3210	−0.0804	0.034*
C10	0.8351 (6)	0.3608 (3)	−0.08061 (10)	0.0302 (7)
H10A	0.8285	0.3725	−0.1125	0.036*
C11	1.0176 (5)	0.3741 (3)	−0.05225 (10)	0.0279 (6)
H11A	1.1344	0.3947	−0.0651	0.034*
C12	1.0296 (4)	0.3571 (2)	−0.00454 (10)	0.0206 (5)
H12A	1.1541	0.3661	0.0142	0.025*
C13	0.8637 (3)	0.4209 (2)	0.14002 (8)	0.0142 (4)
C14	1.0354 (4)	0.4420 (2)	0.17288 (9)	0.0216 (5)
H14A	1.1514	0.3970	0.1734	0.026*
C15	1.0334 (5)	0.5301 (3)	0.20481 (10)	0.0262 (6)
H15A	1.1481	0.5430	0.2264	0.031*
C16	0.8629 (5)	0.5983 (3)	0.20472 (10)	0.0258 (6)
H16A	0.8633	0.6578	0.2257	0.031*
C17	0.6903 (5)	0.5767 (3)	0.17276 (10)	0.0250 (5)
H17A	0.5739	0.6213	0.1728	0.030*
C18	0.6912 (4)	0.4891 (2)	0.14096 (9)	0.0189 (5)
H18A	0.5749	0.4757	0.1199	0.023*
C19	0.3747 (3)	0.2646 (2)	0.09720 (8)	0.0126 (4)
C20	0.3959 (3)	0.1593 (2)	0.12628 (8)	0.0135 (4)
C21	0.4358 (4)	0.1730 (2)	0.17424 (9)	0.0159 (4)
H21A	0.4489	0.2454	0.1867	0.019*
C22	0.4562 (4)	0.0801 (2)	0.20357 (8)	0.0180 (5)
H22A	0.4843	0.0891	0.2356	0.022*
C23	0.4338 (4)	−0.0263 (2)	0.18396 (9)	0.0172 (4)
C24	0.3965 (4)	−0.0443 (2)	0.13664 (9)	0.0161 (4)
H24A	0.3840	−0.1168	0.1242	0.019*
C25	0.3789 (3)	0.0502 (2)	0.10870 (8)	0.0131 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.00987 (7)	0.01279 (7)	0.01270 (7)	0.00097 (5)	0.00238 (5)	0.00141 (5)
O1	0.0082 (7)	0.0209 (8)	0.0193 (8)	0.0007 (6)	0.0048 (6)	0.0025 (7)
O2	0.0104 (7)	0.0169 (8)	0.0226 (9)	0.0018 (6)	0.0059 (6)	−0.0001 (7)
O3	0.0290 (10)	0.0208 (9)	0.0139 (8)	0.0013 (8)	0.0001 (7)	0.0011 (7)
O4	0.0394 (12)	0.0199 (9)	0.0217 (10)	0.0019 (9)	0.0019 (8)	−0.0077 (8)

O5	0.0514 (16)	0.0440 (15)	0.0275 (12)	−0.0072 (12)	−0.0085 (11)	0.0198 (11)
O6	0.0495 (15)	0.0187 (10)	0.0337 (12)	0.0065 (10)	0.0122 (11)	0.0075 (9)
N1	0.0125 (8)	0.0193 (10)	0.0165 (9)	0.0006 (7)	0.0035 (7)	−0.0025 (7)
N2	0.0239 (11)	0.0236 (11)	0.0262 (12)	0.0059 (9)	0.0065 (9)	0.0105 (9)
C1	0.0140 (9)	0.0137 (9)	0.0141 (10)	0.0017 (8)	0.0013 (7)	0.0000 (8)
C2	0.0148 (10)	0.0161 (10)	0.0131 (9)	0.0010 (8)	0.0013 (7)	0.0001 (8)
C3	0.0176 (10)	0.0193 (11)	0.0178 (11)	0.0022 (9)	0.0029 (8)	0.0058 (9)
C4	0.0228 (12)	0.0127 (10)	0.0260 (13)	0.0013 (9)	0.0033 (10)	0.0040 (9)
C5	0.0188 (11)	0.0164 (11)	0.0210 (12)	−0.0010 (9)	0.0054 (9)	−0.0034 (9)
C6	0.0177 (10)	0.0178 (11)	0.0140 (10)	0.0000 (8)	0.0024 (8)	−0.0005 (8)
C7	0.0223 (11)	0.0144 (10)	0.0125 (9)	0.0016 (9)	0.0053 (8)	0.0016 (8)
C8	0.0195 (11)	0.0228 (12)	0.0176 (11)	0.0028 (9)	0.0017 (9)	0.0014 (9)
C9	0.0388 (17)	0.0268 (14)	0.0169 (12)	0.0035 (13)	−0.0024 (11)	0.0021 (10)
C10	0.055 (2)	0.0230 (13)	0.0135 (11)	0.0108 (13)	0.0079 (12)	0.0050 (10)
C11	0.0412 (17)	0.0230 (13)	0.0232 (13)	0.0080 (12)	0.0178 (12)	0.0075 (10)
C12	0.0255 (12)	0.0177 (11)	0.0202 (12)	0.0017 (10)	0.0086 (9)	0.0045 (9)
C13	0.0115 (9)	0.0162 (10)	0.0156 (10)	0.0004 (8)	0.0050 (7)	0.0020 (8)
C14	0.0221 (12)	0.0254 (13)	0.0170 (11)	0.0004 (10)	0.0015 (9)	−0.0049 (9)
C15	0.0318 (15)	0.0299 (14)	0.0166 (11)	−0.0044 (12)	0.0021 (10)	−0.0060 (10)
C16	0.0315 (15)	0.0254 (14)	0.0218 (13)	−0.0005 (11)	0.0084 (11)	−0.0063 (10)
C17	0.0306 (14)	0.0220 (13)	0.0236 (13)	0.0078 (11)	0.0076 (11)	−0.0014 (10)
C18	0.0223 (12)	0.0175 (11)	0.0176 (11)	0.0041 (9)	0.0049 (9)	−0.0010 (9)
C19	0.0104 (9)	0.0134 (9)	0.0137 (9)	−0.0013 (7)	0.0004 (7)	−0.0010 (7)
C20	0.0111 (9)	0.0160 (10)	0.0132 (9)	0.0007 (8)	0.0007 (7)	−0.0003 (8)
C21	0.0144 (10)	0.0176 (10)	0.0155 (10)	0.0006 (8)	0.0010 (8)	−0.0021 (8)
C22	0.0157 (10)	0.0271 (12)	0.0112 (9)	0.0029 (9)	0.0013 (8)	0.0016 (9)
C23	0.0139 (10)	0.0191 (11)	0.0189 (11)	0.0039 (8)	0.0037 (8)	0.0049 (9)
C24	0.0138 (9)	0.0167 (10)	0.0183 (10)	0.0020 (8)	0.0037 (8)	0.0014 (8)
C25	0.0105 (9)	0.0161 (10)	0.0132 (9)	0.0004 (7)	0.0030 (7)	−0.0010 (8)

Geometric parameters (Å, °)

Sn1—C7	2.128 (2)	C9—C10	1.383 (5)
Sn1—C1	2.130 (2)	C9—H9A	0.9300
Sn1—C13	2.136 (2)	C10—C11	1.376 (5)
Sn1—O2^{i}	2.2370 (18)	C10—H10A	0.9300
Sn1—O1	2.2517 (17)	C11—C12	1.391 (4)
O1—C19	1.257 (3)	C11—H11A	0.9300
O2—C19	1.252 (3)	C12—H12A	0.9300
O2—Sn1^{ii}	2.2370 (18)	C13—C18	1.397 (3)
O3—N1	1.223 (3)	C13—C14	1.405 (3)
O4—N1	1.219 (3)	C14—C15	1.396 (4)
O5—N2	1.230 (3)	C14—H14A	0.9300
O6—N2	1.224 (3)	C15—C16	1.383 (4)
N1—C25	1.482 (3)	C15—H15A	0.9300
N2—C23	1.463 (3)	C16—C17	1.396 (4)
C1—C2	1.400 (3)	C16—H16A	0.9300
C1—C6	1.406 (3)	C17—C18	1.388 (4)
C2—C3	1.398 (4)	C17—H17A	0.9300

C2—H2A	0.9300	C18—H18A	0.9300
C3—C4	1.392 (4)	C19—C20	1.502 (3)
C3—H3A	0.9300	C20—C25	1.388 (3)
C4—C5	1.385 (4)	C20—C21	1.392 (3)
C4—H4A	0.9300	C21—C22	1.387 (4)
C5—C6	1.400 (4)	C21—H21A	0.9300
C5—H5A	0.9300	C22—C23	1.382 (4)
C6—H6A	0.9300	C22—H22A	0.9300
C7—C12	1.396 (4)	C23—C24	1.380 (4)
C7—C8	1.397 (4)	C24—C25	1.378 (3)
C8—C9	1.390 (4)	C24—H24A	0.9300
C8—H8A	0.9300		
C7—Sn1—C1	115.46 (9)	C9—C10—H10A	120.3
C7—Sn1—C13	124.90 (9)	C10—C11—C12	120.9 (3)
C1—Sn1—C13	119.61 (9)	C10—C11—H11A	119.6
C7—Sn1—O2^{i}	89.85 (9)	C12—C11—H11A	119.6
C1—Sn1—O2^{i}	95.25 (8)	C11—C12—C7	120.1 (3)
C13—Sn1—O2^{i}	87.22 (8)	C11—C12—H12A	119.9
C7—Sn1—O1	87.89 (9)	C7—C12—H12A	119.9
C1—Sn1—O1	93.78 (8)	C18—C13—C14	118.0 (2)
C13—Sn1—O1	86.75 (8)	C18—C13—Sn1	120.80 (18)
O2^{i}—Sn1—O1	170.79 (7)	C14—C13—Sn1	121.12 (18)
C19—O1—Sn1	142.06 (16)	C15—C14—C13	120.6 (3)
C19—O2—Sn1^{ii}	141.46 (17)	C15—C14—H14A	119.7
O4—N1—O3	125.3 (2)	C13—C14—H14A	119.7
O4—N1—C25	117.7 (2)	C16—C15—C14	120.8 (3)
O3—N1—C25	117.0 (2)	C16—C15—H15A	119.6
O6—N2—O5	124.1 (3)	C14—C15—H15A	119.6
O6—N2—C23	118.6 (2)	C15—C16—C17	119.1 (3)
O5—N2—C23	117.3 (3)	C15—C16—H16A	120.4
C2—C1—C6	118.8 (2)	C17—C16—H16A	120.4
C2—C1—Sn1	122.94 (18)	C18—C17—C16	120.4 (3)
C6—C1—Sn1	118.29 (17)	C18—C17—H17A	119.8
C3—C2—C1	120.3 (2)	C16—C17—H17A	119.8
C3—C2—H2A	119.9	C17—C18—C13	121.2 (3)
C1—C2—H2A	119.9	C17—C18—H18A	119.4
C4—C3—C2	120.5 (2)	C13—C18—H18A	119.4
C4—C3—H3A	119.8	O2—C19—O1	122.6 (2)
C2—C3—H3A	119.8	O2—C19—C20	117.9 (2)
C5—C4—C3	119.8 (2)	O1—C19—C20	119.1 (2)
C5—C4—H4A	120.1	C25—C20—C21	118.2 (2)
C3—C4—H4A	120.1	C25—C20—C19	124.6 (2)
C4—C5—C6	120.2 (2)	C21—C20—C19	117.2 (2)
C4—C5—H5A	119.9	C22—C21—C20	120.8 (2)
C6—C5—H5A	119.9	C22—C21—H21A	119.6
C5—C6—C1	120.5 (2)	C20—C21—H21A	119.6
C5—C6—H6A	119.8	C23—C22—C21	118.2 (2)
C1—C6—H6A	119.8	C23—C22—H22A	120.9

C12—C7—C8	118.6 (2)	C21—C22—H22A	120.9
C12—C7—Sn1	120.95 (19)	C24—C23—C22	123.1 (2)
C8—C7—Sn1	120.4 (2)	C24—C23—N2	118.4 (2)
C9—C8—C7	120.5 (3)	C22—C23—N2	118.5 (2)
C9—C8—H8A	119.8	C25—C24—C23	116.8 (2)
C7—C8—H8A	119.8	C25—C24—H24A	121.6
C10—C9—C8	120.5 (3)	C23—C24—H24A	121.6
C10—C9—H9A	119.8	C24—C25—C20	122.9 (2)
C8—C9—H9A	119.8	C24—C25—N1	117.8 (2)
C11—C10—C9	119.4 (3)	C20—C25—N1	119.4 (2)
C11—C10—H10A	120.3		
C7—Sn1—O1—C19	154.9 (3)	C1—Sn1—C13—C14	69.1 (2)
C1—Sn1—O1—C19	39.5 (3)	$O2^{i}$—Sn1—C13—C14	−25.4 (2)
C13—Sn1—O1—C19	−80.0 (3)	O1—Sn1—C13—C14	161.6 (2)
C7—Sn1—C1—C2	173.48 (19)	C18—C13—C14—C15	−1.1 (4)
C13—Sn1—C1—C2	−8.6 (2)	Sn1—C13—C14—C15	175.6 (2)
$O2^{i}$—Sn1—C1—C2	81.1 (2)	C13—C14—C15—C16	−0.1 (5)
O1—Sn1—C1—C2	−97.1 (2)	C14—C15—C16—C17	1.2 (5)
C7—Sn1—C1—C6	−6.7 (2)	C15—C16—C17—C18	−1.1 (5)
C13—Sn1—C1—C6	171.17 (17)	C16—C17—C18—C13	−0.1 (4)
$O2^{i}$—Sn1—C1—C6	−99.04 (19)	C14—C13—C18—C17	1.2 (4)
O1—Sn1—C1—C6	82.76 (19)	Sn1—C13—C18—C17	−175.5 (2)
C6—C1—C2—C3	0.7 (4)	$Sn1^{ii}$—O2—C19—O1	143.0 (2)
Sn1—C1—C2—C3	−179.48 (18)	$Sn1^{ii}$—O2—C19—C20	−43.6 (4)
C1—C2—C3—C4	−0.9 (4)	Sn1—O1—C19—O2	149.4 (2)
C2—C3—C4—C5	0.4 (4)	Sn1—O1—C19—C20	−23.9 (4)
C3—C4—C5—C6	0.4 (4)	O2—C19—C20—C25	103.4 (3)
C4—C5—C6—C1	−0.6 (4)	O1—C19—C20—C25	−83.0 (3)
C2—C1—C6—C5	0.0 (4)	O2—C19—C20—C21	−76.7 (3)
Sn1—C1—C6—C5	−179.79 (19)	O1—C19—C20—C21	96.9 (3)
C1—Sn1—C7—C12	−99.5 (2)	C25—C20—C21—C22	−0.5 (4)
C13—Sn1—C7—C12	82.8 (2)	C19—C20—C21—C22	179.6 (2)
$O2^{i}$—Sn1—C7—C12	−3.7 (2)	C20—C21—C22—C23	−0.7 (4)
O1—Sn1—C7—C12	167.3 (2)	C21—C22—C23—C24	1.5 (4)
C1—Sn1—C7—C8	77.5 (2)	C21—C22—C23—N2	−178.6 (2)
C13—Sn1—C7—C8	−100.2 (2)	O6—N2—C23—C24	−17.0 (4)
$O2^{i}$—Sn1—C7—C8	173.3 (2)	O5—N2—C23—C24	163.3 (3)
O1—Sn1—C7—C8	−15.7 (2)	O6—N2—C23—C22	163.1 (3)
C12—C7—C8—C9	−0.8 (4)	O5—N2—C23—C22	−16.7 (4)
Sn1—C7—C8—C9	−177.8 (2)	C22—C23—C24—C25	−1.0 (4)
C7—C8—C9—C10	0.4 (4)	N2—C23—C24—C25	179.1 (2)
C8—C9—C10—C11	0.0 (5)	C23—C24—C25—C20	−0.3 (4)
C9—C10—C11—C12	−0.1 (5)	C23—C24—C25—N1	179.5 (2)
C10—C11—C12—C7	−0.3 (4)	C21—C20—C25—C24	1.0 (4)
C8—C7—C12—C11	0.7 (4)	C19—C20—C25—C24	−179.1 (2)
Sn1—C7—C12—C11	177.7 (2)	C21—C20—C25—N1	−178.8 (2)
C7—Sn1—C13—C18	63.3 (2)	C19—C20—C25—N1	1.1 (3)

C1—Sn1—C13—C18	−114.3 (2)	O4—N1—C25—C24	−12.5 (3)
O2^{i}—Sn1—C13—C18	151.2 (2)	O3—N1—C25—C24	165.9 (2)
O1—Sn1—C13—C18	−21.8 (2)	O4—N1—C25—C20	167.4 (2)
C7—Sn1—C13—C14	−113.3 (2)	O3—N1—C25—C20	−14.2 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8A···O1	0.93	2.37	2.977 (3)	123
C18—H18A···O1	0.93	2.39	2.984 (3)	121
C12—H12A···O2^{i}	0.93	2.40	3.026 (3)	124
C14—H14A···O2^{i}	0.93	2.52	3.028 (3)	115
C17—H17A···O6^{iii}	0.93	2.47	3.331 (4)	153
C21—H21A···O5^{iv}	0.93	2.40	3.279 (3)	158

Symmetry codes: (i) *x*+1, *y*, *z*; (iii) *x*, *y*+1, *z*; (iv) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

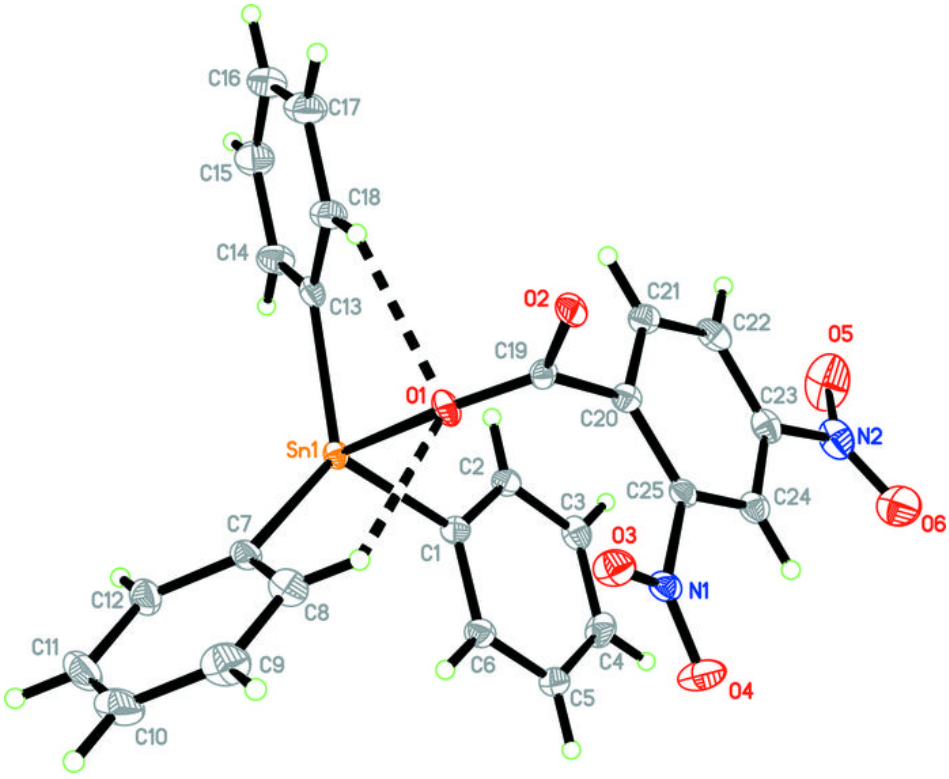
C16
C17
C15
C18
C14
C13
O2
C21
C22
O5
C19
O1
C23
C20
N2
Sn1
C2
C25
C24
O6
C3
C7
C1
O3
N1
C12
C8
C11
C9
C6
C4
O4
C5
C10

Fig. 2