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{(*E*)-4-[(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)imino-methyl]benzoato}triphenyltin(IV)

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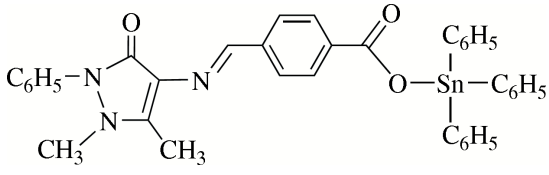
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.023; wR factor = 0.060; data-to-parameter ratio = 13.5.

The title compound, $[Sn(C_6H_5)_3(C_{19}H_{16}N_3O_3)]$, is a four-coordinate Sn^{IV} complex, with a distorted tetrahedral geometry and one disordered (0.54:0.46) phenyl ring. The Schiff base carboxylate group acts as a monodentate ligand coordinating through the deprotonated hydroxyl O atom. In the crystal structure, a weak offset face-to-face aromatic π–π stacking interaction can be found between the pyrazole ring and the benzene ring of 4-formylbenzoic acid. The centroid-to-centroid distance is 3.858 (2) Å and the interplanar distance is 3.375 (4) Å.

Related literature

For related literature, see: Barbieri *et al.* (2001); Fang *et al.* (2001); Fang *et al.* (2006); Hu *et al.* (2006); Hökelek *et al.* (2002); Ma *et al.* (2005); Zhou *et al.* (2005).



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_{19}H_{16}N_3O_3)]$
M_r = 684.34
Triclinic, $P\overline{1}$
a = 9.2009 (14) Å
b = 12.6299 (19) Å
c = 15.598 (2) Å
α = 74.435 (2)°
β = 77.913 (2)°
γ = 68.677 (2)°
V = 1613.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 296 (2) K
0.41 × 0.39 × 0.31 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.727, T_{max} = 0.783
9137 measured reflections
5246 independent reflections
5039 reflections with $I > 2\sigma(I)$
R_{int} = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.04
5246 reflections
388 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C32—Sn1	2.126 (2)	C19—O1	1.311 (3)
C32*A*—Sn1	2.199 (2)	C20—Sn1	2.122 (2)
C11—O3	1.228 (3)	C26—Sn1	2.119 (2)
C12—N1	1.271 (3)	O1—Sn1	2.044 (2)
C19—O2	1.216 (3)		
O2—C19—O1	122.9 (2)	C26—Sn1—C20	116.41 (9)
C19—O1—Sn1	117.4 (2)	O1—Sn1—C32	91.00 (8)
O1—Sn1—C26	111.39 (8)	C26—Sn1—C32	110.05 (8)
O1—Sn1—C20	107.81 (8)	C20—Sn1—C32	117.23 (8)

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2019).

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supplementary materials

Acta Cryst. (2007). E**63**, m1843 [**doi:10.1107/S1600536807027298**]

{(*E*)-4-[(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)iminomethyl]benzoato}triphenyltin(IV)

X.-N. Fang, Y. Sui, R.-H. Hu, Q.-Y. Luo and H.-Q. Qin

Comment

4-aminoantipyrine and its derivatives are important compounds in pharmacology and biochemistry. They are especially used as anti-inflammatory drugs (Hökelek *et al.*, 2002). The structural chemistry of organotin carboxylate complexs has attracted considerable attention, owing to their good antitumor activities (Barbieri *et al.*, 2001; Zhou *et al.*, 2005), their versatile molecular structures and the supramolecular architectures exhibited by these complexes (Ma *et al.*, 2005). In the context of our continued interest in the structural and biological properties of organotin complexes (Fang *et al.*, 2001; Fang, *et al.*, 2006), we have been interested in studying the biologigal properties of the title compound.

The title compound (*E*)-4-[(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-ylimino)methyl] benzoato-triphenyltin (IV), is a four-coordinate Sn^{IV} complex, with a distorted tetrahedron geometry (Fig. 1). The (*E*)-4-((1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-ylimino)methyl) benzoate ligand, coordinates in monodentate mode bonding with the triphenyltin group. The Sn1—O1 bond length is 2.044 (2) Å, which is slightly shorter than the value of 2.121 (3)Å reported by Fang, Sui *et al.* (2006*a*). The double bond C═ N length is 1.271 (3) Å, and this is comparable to the analogue of 1.280 (3)Å found by Hu *et al.* (2006).

The ring of pyrazole is well coplanar, with a mean deviation from the plane of 0.027 (3) Å, and makes an angle of 49.9 (2)° with the substituent phenyl (C1 to C6) and 20.7 (2)° with the benzene ring of 4-formylbenzoic acid (C13 to C18).

In the crystal lattice (Fig. 2), a weak aromatic π-π stacking interaction can be found between the pyrazole ring (*Cg*1) and benzene ring (*Cg*2) of 4-formylbenzoic acid [the distance of $Cg1\cdots Cg2^{i}$ is 3.858 (2) Å; and the $C10\cdots C18^{i}$ distance in the offset face-to-face interaction is 3.375 (4) Å; symmetry code: (i) $1-x, 1-y, -z$)].

Experimental

The title compound (I) was prepared by the following procedure: A solution of Schiff base ligand, (*E*)-4-((1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-ylimino)methyl)\ benzoic acid, (0.335 g, 1 m mol) and triphenyltin hydroxide (0.367 g, 1 mmol) in 20 ml mixed solvent (benzene:toluene = 1:1) was heated for 6 h under reflux. The solvent was removed by vacuum distillation in a rotary evaporator and a yellow solid product was obtained (yield 83%, m.p. 497–498 K). When the solid was recrystallized from toluene, single crystals suitable for X-ray diffraction analysis precipitated after several days.

Refinement

One phenyl ring of the triphenyltin is disordered in the crystal structure. Each of the six atoms can be splitted into two parts to form two six-membered rings, and the positional occupancy factors is 0.54. A l l the H atoms were positioned in idealized locations and refined as riding on their carrier atoms, with C—H distances of 0.93 (aryl) and 0.96Å (methyl) with U_{iso}(H) = 1.5Ueq(C) for methyl and U_{iso}(H) = 1.2Ueq(C) for aryl.

Figures

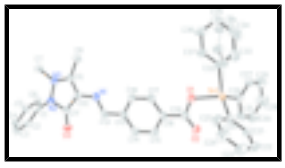


Fig.1. Molecular structure of (I), showing 30% probability displacement ellipsoids. All the H atoms have been omitted for clarity.

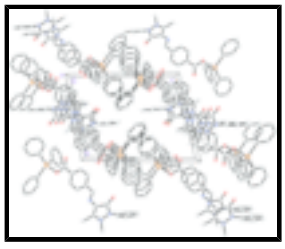


Fig.2. The packing diagram of (I), viewed down the *a* axis. All the H atoms and part of the disordered phenyl have been omitted for clarity.

Table 1. Selected geometric parameters (Å, °).

{(*E*)-4-[(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)iminomethyl]\ benzoato}triphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_{19}H_{16}N_3O_3)]$	$Z = 2$
$M_r = 684.34$	$F_{000} = 696$
Triclinic, $P\overline{1}$	$D_x = 1.408$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 497-498 K
$a = 9.2009$ (14) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 12.6299$ (19) Å	Cell parameters from 5058 reflections
$c = 15.598$ (2) Å	$\theta = 2.4$–29.2º
$\alpha = 74.435$ (2)º	$\mu = 0.83$ mm^{-1}
$\beta = 77.913$ (2)º	$T = 296$ (2) K
$\gamma = 68.677$ (2)º	Block, yellow
$V = 1613.9$ (4) Å^3	0.41 × 0.39 × 0.31 mm

Data collection

Bruker APEX II area-detector diffractometer	5246 independent reflections
Radiation source: fine-focus sealed tube	5039 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.011$
$T = 296$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -10 \rightarrow 10$
$T_{min} = 0.727$, $T_{max} = 0.783$	$k = -15 \rightarrow 14$
9137 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.060$

$S = 1.04$

5246 reflections

388 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.6678P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.37$ e Å^{-3}

$\Delta\rho_{min} = -0.27$ e Å^{-3}

Extinction correction: none

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 $F^2 > 2$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}	Occ. (<1)
C32	0.5054 (2)	0.77153 (16)	0.45208 (11)	0.0465 (6)	0.536 (3)
C33	0.5808 (2)	0.75898 (14)	0.52445 (12)	0.0605 (9)	0.536 (3)
H33	0.6272	0.8132	0.5246	0.073*	0.536 (3)
C34	0.5868 (3)	0.66540 (18)	0.59664 (11)	0.0714 (13)	0.536 (3)
H34	0.6372	0.6570	0.6451	0.086*	0.536 (3)
C35	0.5174 (3)	0.58438 (18)	0.59645 (17)	0.0784 (16)	0.536 (3)
H35	0.5214	0.5218	0.6448	0.094*	0.536 (3)
C36	0.4420 (4)	0.5969 (2)	0.5241 (2)	0.0808 (13)	0.536 (3)
H36	0.3956	0.5427	0.5240	0.097*	0.536 (3)
C37	0.4360 (3)	0.6905 (2)	0.45190 (17)	0.0650 (10)	0.536 (3)
H37	0.3856	0.6989	0.4035	0.078*	0.536 (3)
C32A	0.5064 (2)	0.78462 (14)	0.46971 (11)	0.0465 (6)	0.464 (3)
C33A	0.6317 (3)	0.75826 (18)	0.51712 (14)	0.0605 (9)	0.464 (3)
H33A	0.7072	0.7952	0.4966	0.073*	0.464 (3)
C34A	0.6397 (3)	0.6752 (2)	0.59586 (13)	0.0714 (13)	0.464 (3)
H34A	0.7250	0.6517	0.6276	0.086*	0.464 (3)
C35A	0.5229 (3)	0.6275 (2)	0.62702 (12)	0.0784 (16)	0.464 (3)
H35A	0.5295	0.5711	0.6798	0.094*	0.464 (3)
C36A	0.3992 (3)	0.6606 (2)	0.58286 (17)	0.0808 (13)	0.464 (3)
H36A	0.3179	0.6299	0.6064	0.097*	0.464 (3)
C37A	0.39118 (18)	0.7403 (2)	0.50232 (16)	0.0650 (10)	0.464 (3)
H37A	0.3053	0.7627	0.4712	0.078*	0.464 (3)

C1	0.1119 (2)	0.41572 (17)	−0.22321 (13)	0.0423 (4)
C2	0.2001 (3)	0.4252 (2)	−0.30692 (14)	0.0501 (5)
H2	0.3011	0.4287	−0.3130	0.060*
C3	0.1371 (3)	0.4295 (2)	−0.38092 (15)	0.0584 (6)
H3	0.1951	0.4378	−0.4374	0.070*
C4	−0.0104 (3)	0.4217 (2)	−0.37211 (16)	0.0655 (7)
H4	−0.0517	0.4234	−0.4222	0.079*
C5	−0.0974 (3)	0.4114 (2)	−0.28821 (17)	0.0633 (6)
H5	−0.1971	0.4055	−0.2820	0.076*
C6	−0.0374 (3)	0.4097 (2)	−0.21355 (15)	0.0512 (5)
H6	−0.0970	0.4047	−0.1575	0.061*
C7	0.1644 (3)	0.2264 (2)	−0.05646 (17)	0.0622 (6)
H7A	0.2691	0.1866	−0.0808	0.093*
H7B	0.0899	0.2224	−0.0894	0.093*
H7C	0.1455	0.1903	0.0055	0.093*
C8	0.1921 (4)	0.3250 (2)	0.09253 (16)	0.0676 (7)
H8A	0.0927	0.3131	0.1156	0.101*
H8B	0.2105	0.3709	0.1267	0.101*
H8C	0.2743	0.2511	0.0971	0.101*
C9	0.1902 (3)	0.38690 (19)	−0.00328 (14)	0.0471 (5)
C10	0.2312 (2)	0.48386 (19)	−0.04414 (13)	0.0444 (5)
C11	0.2225 (3)	0.50515 (19)	−0.13904 (14)	0.0467 (5)
C12	0.3037 (3)	0.6390 (2)	−0.03608 (15)	0.0546 (5)
H12	0.3023	0.6662	−0.0976	0.066*
C13	0.3429 (3)	0.7033 (2)	0.01676 (15)	0.0511 (5)
C14	0.3378 (4)	0.8184 (2)	−0.01735 (17)	0.0685 (7)
H14	0.3169	0.8535	−0.0760	0.082*
C15	0.3635 (3)	0.8807 (2)	0.03530 (17)	0.0665 (7)
H15	0.3582	0.9578	0.0120	0.080*
C16	0.3970 (3)	0.8293 (2)	0.12243 (14)	0.0487 (5)
C17	0.4097 (3)	0.7134 (2)	0.15472 (15)	0.0503 (5)
H17	0.4363	0.6772	0.2123	0.060*
C18	0.3834 (3)	0.6508 (2)	0.10266 (15)	0.0503 (5)
H18	0.3929	0.5729	0.1254	0.060*
C19	0.4175 (3)	0.8982 (2)	0.18055 (15)	0.0540 (6)
C20	0.6833 (3)	0.97250 (19)	0.29455 (14)	0.0477 (5)
C21	0.6816 (3)	1.0830 (2)	0.29179 (17)	0.0617 (6)
H21	0.5893	1.1371	0.3116	0.074*
C22	0.8154 (4)	1.1144 (3)	0.2600 (2)	0.0774 (8)
H22	0.8132	1.1889	0.2590	0.093*
C23	0.9509 (4)	1.0356 (3)	0.2300 (2)	0.0861 (9)
H23	1.0409	1.0565	0.2085	0.103*
C24	0.9544 (4)	0.9259 (3)	0.2316 (3)	0.0909 (10)
H24	1.0465	0.8726	0.2107	0.109*
C25	0.8211 (3)	0.8941 (2)	0.2643 (2)	0.0686 (7)
H25	0.8244	0.8192	0.2659	0.082*
C26	0.2702 (3)	1.0560 (2)	0.37759 (14)	0.0498 (5)
C27	0.1939 (3)	1.0432 (2)	0.46467 (17)	0.0641 (6)
H27	0.2324	0.9752	0.5066	0.077*

C28	0.0620 (4)	1.1302 (3)	0.4896 (2)	0.0955 (11)
H28	0.0106	1.1209	0.5478	0.115*
C29	0.0069 (5)	1.2307 (3)	0.4277 (3)	0.1140 (14)
H29	−0.0814	1.2900	0.4447	0.137*
C30	0.0794 (5)	1.2453 (3)	0.3415 (3)	0.1008 (11)
H30	0.0401	1.3136	0.3001	0.121*
C31	0.2119 (3)	1.1576 (2)	0.31647 (18)	0.0697 (7)
H31	0.2619	1.1673	0.2580	0.084*
N1	0.2718 (2)	0.54639 (17)	0.00252 (12)	0.0485 (4)
N2	0.1793 (2)	0.41422 (16)	−0.14869 (11)	0.0467 (4)
N3	0.1472 (2)	0.34757 (15)	−0.06359 (11)	0.0466 (4)
O1	0.4520 (2)	0.83730 (15)	0.26047 (11)	0.0618 (4)
O2	0.4028 (3)	1.00110 (17)	0.15681 (13)	0.0770 (5)
O3	0.2441 (2)	0.58297 (16)	−0.20178 (11)	0.0671 (5)
Sn1	0.480454 (17)	0.922187 (12)	0.347192 (9)	0.04610 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C32	0.0509 (13)	0.0475 (15)	0.0381 (14)	−0.0128 (11)	−0.0024 (10)	−0.0110 (11)
C33	0.078 (3)	0.0494 (16)	0.0603 (16)	−0.0201 (16)	−0.0200 (17)	−0.0135 (13)
C34	0.086 (3)	0.064 (2)	0.0606 (18)	−0.010 (2)	−0.0268 (19)	−0.0137 (15)
C35	0.084 (3)	0.063 (3)	0.073 (3)	−0.024 (2)	−0.013 (2)	0.013 (2)
C36	0.080 (3)	0.069 (3)	0.094 (3)	−0.046 (2)	−0.015 (2)	0.014 (2)
C37	0.062 (2)	0.069 (3)	0.066 (3)	−0.034 (2)	−0.0151 (19)	0.0047 (17)
C32A	0.0509 (13)	0.0475 (15)	0.0381 (14)	−0.0128 (11)	−0.0024 (10)	−0.0110 (11)
C33A	0.078 (3)	0.0494 (16)	0.0603 (16)	−0.0201 (16)	−0.0200 (17)	−0.0135 (13)
C34A	0.086 (3)	0.064 (2)	0.0606 (18)	−0.010 (2)	−0.0268 (19)	−0.0137 (15)
C35A	0.084 (3)	0.063 (3)	0.073 (3)	−0.024 (2)	−0.013 (2)	0.013 (2)
C36A	0.080 (3)	0.069 (3)	0.094 (3)	−0.046 (2)	−0.015 (2)	0.014 (2)
C37A	0.062 (2)	0.069 (3)	0.066 (3)	−0.034 (2)	−0.0151 (19)	0.0047 (17)
C1	0.0539 (12)	0.0341 (11)	0.0399 (10)	−0.0141 (9)	−0.0064 (8)	−0.0091 (8)
C2	0.0547 (12)	0.0479 (13)	0.0464 (12)	−0.0179 (10)	−0.0017 (9)	−0.0096 (10)
C3	0.0740 (16)	0.0575 (15)	0.0398 (11)	−0.0196 (12)	−0.0017 (10)	−0.0108 (10)
C4	0.0819 (18)	0.0727 (18)	0.0473 (13)	−0.0246 (14)	−0.0194 (12)	−0.0137 (12)
C5	0.0586 (14)	0.0754 (18)	0.0614 (15)	−0.0252 (13)	−0.0145 (11)	−0.0133 (13)
C6	0.0535 (12)	0.0548 (14)	0.0445 (11)	−0.0184 (10)	0.0000 (9)	−0.0128 (10)
C7	0.0867 (18)	0.0441 (14)	0.0575 (14)	−0.0269 (12)	−0.0085 (12)	−0.0063 (11)
C8	0.097 (2)	0.0619 (17)	0.0429 (12)	−0.0285 (14)	−0.0115 (12)	−0.0043 (11)
C9	0.0529 (12)	0.0458 (13)	0.0389 (10)	−0.0128 (10)	−0.0045 (9)	−0.0086 (9)
C10	0.0465 (11)	0.0453 (12)	0.0418 (11)	−0.0138 (9)	−0.0041 (8)	−0.0123 (9)
C11	0.0553 (12)	0.0453 (13)	0.0443 (11)	−0.0217 (10)	−0.0055 (9)	−0.0104 (10)
C12	0.0660 (14)	0.0589 (15)	0.0458 (12)	−0.0255 (12)	−0.0063 (10)	−0.0155 (11)
C13	0.0546 (12)	0.0557 (14)	0.0498 (12)	−0.0232 (11)	−0.0011 (9)	−0.0188 (10)
C14	0.105 (2)	0.0661 (17)	0.0467 (13)	−0.0423 (15)	−0.0147 (13)	−0.0075 (12)
C15	0.098 (2)	0.0545 (15)	0.0580 (14)	−0.0390 (14)	−0.0117 (13)	−0.0087 (12)
C16	0.0505 (12)	0.0531 (14)	0.0484 (12)	−0.0216 (10)	−0.0002 (9)	−0.0181 (10)
C17	0.0507 (12)	0.0549 (14)	0.0496 (12)	−0.0182 (10)	−0.0080 (9)	−0.0152 (10)

C18	0.0507 (12)	0.0480 (13)	0.0562 (13)	−0.0178 (10)	−0.0076 (10)	−0.0146 (10)
C19	0.0579 (13)	0.0596 (16)	0.0527 (13)	−0.0262 (11)	0.0015 (10)	−0.0215 (11)
C20	0.0576 (13)	0.0477 (13)	0.0417 (11)	−0.0233 (10)	−0.0057 (9)	−0.0077 (9)
C21	0.0731 (16)	0.0491 (14)	0.0647 (15)	−0.0231 (12)	−0.0063 (12)	−0.0123 (11)
C22	0.100 (2)	0.0607 (18)	0.086 (2)	−0.0478 (17)	−0.0129 (16)	−0.0063 (15)
C23	0.0746 (19)	0.095 (2)	0.098 (2)	−0.0501 (19)	0.0008 (16)	−0.0129 (19)
C24	0.0642 (18)	0.083 (2)	0.122 (3)	−0.0289 (16)	0.0144 (17)	−0.031 (2)
C25	0.0681 (16)	0.0535 (16)	0.0856 (18)	−0.0238 (13)	0.0043 (13)	−0.0218 (13)
C26	0.0600 (13)	0.0457 (13)	0.0468 (12)	−0.0193 (10)	−0.0061 (10)	−0.0125 (10)
C27	0.0788 (17)	0.0548 (15)	0.0576 (14)	−0.0278 (13)	0.0038 (12)	−0.0113 (12)
C28	0.105 (2)	0.076 (2)	0.088 (2)	−0.0301 (19)	0.0373 (19)	−0.0272 (18)
C29	0.100 (3)	0.070 (2)	0.131 (3)	0.0009 (19)	0.029 (2)	−0.027 (2)
C30	0.110 (3)	0.058 (2)	0.098 (3)	0.0032 (18)	−0.008 (2)	−0.0051 (17)
C31	0.0848 (18)	0.0567 (16)	0.0538 (14)	−0.0108 (14)	−0.0067 (12)	−0.0081 (12)
N1	0.0516 (10)	0.0518 (11)	0.0460 (10)	−0.0171 (9)	−0.0046 (8)	−0.0176 (8)
N2	0.0629 (11)	0.0457 (11)	0.0360 (9)	−0.0258 (9)	−0.0069 (7)	−0.0041 (7)
N3	0.0629 (11)	0.0388 (10)	0.0386 (9)	−0.0204 (8)	−0.0059 (8)	−0.0041 (7)
O1	0.0841 (12)	0.0599 (11)	0.0540 (9)	−0.0310 (9)	−0.0121 (8)	−0.0193 (8)
O2	0.1188 (16)	0.0598 (12)	0.0684 (11)	−0.0432 (11)	−0.0131 (11)	−0.0185 (9)
O3	0.1088 (14)	0.0638 (11)	0.0454 (9)	−0.0542 (10)	−0.0106 (9)	−0.0012 (8)
Sn1	0.05547 (10)	0.04475 (10)	0.04128 (9)	−0.02024 (7)	−0.00573 (6)	−0.00908 (6)

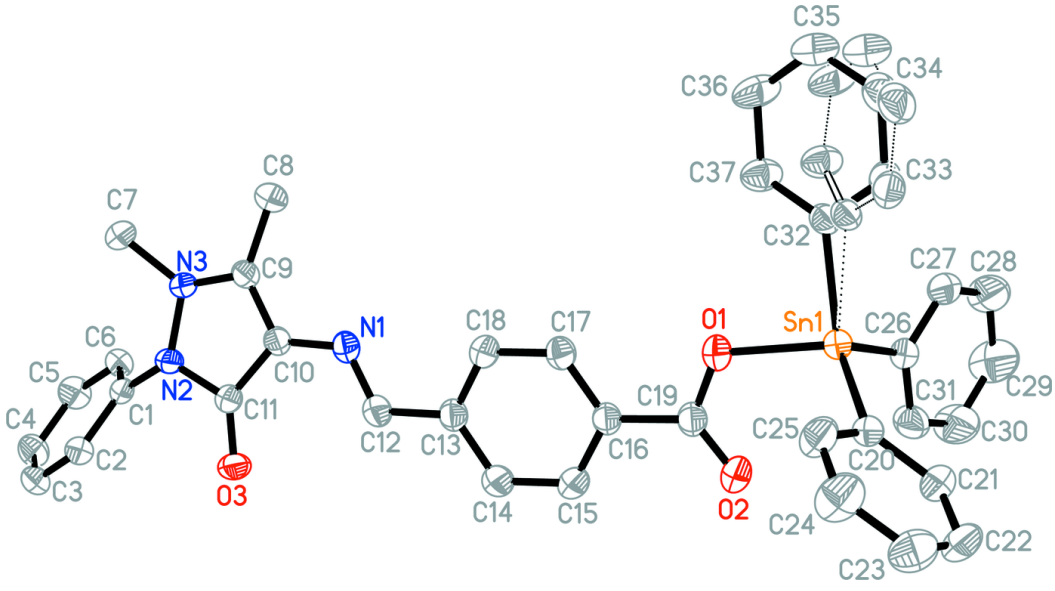
Geometric parameters (Å, °)

C32—C33	1.3900	C10—N1	1.389 (3)
C32—C37	1.3900	C10—C11	1.446 (3)
C32—Sn1	2.126 (2)	C11—O3	1.228 (3)
C33—C34	1.3900	C11—N2	1.396 (3)
C33—H33	0.93	C12—N1	1.271 (3)
C34—C35	1.3900	C12—C13	1.471 (3)
C34—H34	0.93	C12—H12	0.93
C35—C36	1.3900	C13—C18	1.388 (3)
C35—H35	0.93	C13—C14	1.394 (4)
C36—C37	1.3900	C14—C15	1.384 (4)
C36—H36	0.93	C14—H14	0.93
C37—H37	0.93	C15—C16	1.386 (3)
C32A—C37A	1.3224	C15—H15	0.93
C32A—C33A	1.3900	C16—C17	1.384 (3)
C32A—Sn1	2.199 (2)	C16—C19	1.493 (3)
C33A—C34A	1.3802	C17—C18	1.382 (3)
C33A—H33A	0.93	C17—H17	0.93
C34A—C35A	1.3592	C18—H18	0.93
C34A—H34A	0.93	C19—O2	1.216 (3)
C35A—C36A	1.3313	C19—O1	1.311 (3)
C35A—H35A	0.93	C20—C25	1.377 (3)
C36A—C37A	1.3792	C20—C21	1.379 (3)
C36A—H36A	0.93	C20—Sn1	2.122 (2)
C37A—H37A	0.93	C21—C22	1.382 (4)
C1—C6	1.377 (3)	C21—H21	0.9300

C1—C2	1.386 (3)	C22—C23	1.366 (5)
C1—N2	1.421 (3)	C22—H22	0.93
C2—C3	1.376 (3)	C23—C24	1.367 (5)
C2—H2	0.93	C23—H23	0.93
C3—C4	1.372 (4)	C24—C25	1.382 (4)
C3—H3	0.93	C24—H24	0.93
C4—C5	1.384 (4)	C25—H25	0.93
C4—H4	0.93	C26—C31	1.379 (3)
C5—C6	1.382 (3)	C26—C27	1.389 (3)
C5—H5	0.93	C26—Sn1	2.119 (2)
C6—H6	0.93	C27—C28	1.376 (4)
C7—N3	1.456 (3)	C27—H27	0.93
C7—H7A	0.96	C28—C29	1.370 (5)
C7—H7B	0.96	C28—H28	0.93
C7—H7C	0.96	C29—C30	1.367 (5)
C8—C9	1.490 (3)	C29—H29	0.93
C8—H8A	0.96	C30—C31	1.384 (4)
C8—H8B	0.96	C30—H30	0.93
C8—H8C	0.96	C31—H31	0.93
C9—N3	1.356 (3)	N2—N3	1.405 (2)
C9—C10	1.366 (3)	O1—Sn1	2.044 (2)
C33—C32—C37	120.0	C13—C12—H12	120.0
C33—C32—Sn1	119.62 (10)	C18—C13—C14	118.5 (2)
C37—C32—Sn1	120.19 (10)	C18—C13—C12	120.4 (2)
C32—C33—C34	120.0	C14—C13—C12	121.1 (2)
C32—C33—H33	120.0	C15—C14—C13	120.6 (2)
C34—C33—H33	120.0	C15—C14—H14	119.7
C33—C34—C35	120.0	C13—C14—H14	119.7
C33—C34—H34	120.0	C14—C15—C16	120.6 (2)
C35—C34—H34	120.0	C14—C15—H15	119.7
C34—C35—C36	120.0	C16—C15—H15	119.7
C34—C35—H35	120.0	C17—C16—C15	118.8 (2)
C36—C35—H35	120.0	C17—C16—C19	120.7 (2)
C37—C36—C35	120.0	C15—C16—C19	120.5 (2)
C37—C36—H36	120.0	C18—C17—C16	120.9 (2)
C35—C36—H36	120.0	C18—C17—H17	119.5
C36—C37—C32	120.0	C16—C17—H17	119.5
C36—C37—H37	120.0	C17—C18—C13	120.5 (2)
C32—C37—H37	120.0	C17—C18—H18	119.7
C37A—C32A—C33A	121.6	C13—C18—H18	119.7
C37A—C32A—Sn1	118.54 (10)	O2—C19—O1	122.9 (2)
C33A—C32A—Sn1	119.23 (10)	O2—C19—C16	123.6 (2)
C34A—C33A—C32A	117.4	O1—C19—C16	113.5 (2)
C34A—C33A—H33A	121.3	C25—C20—C21	118.5 (2)
C32A—C33A—H33A	121.3	C25—C20—Sn1	120.44 (18)
C35A—C34A—C33A	120.1	C21—C20—Sn1	121.00 (18)
C35A—C34A—H34A	120.0	C20—C21—C22	120.8 (3)
C33A—C34A—H34A	120.0	C20—C21—H21	119.6
C36A—C35A—C34A	120.8	C22—C21—H21	119.6

C36A—C35A—H35A	119.6	C23—C22—C21	119.8 (3)
C34A—C35A—H35A	119.6	C23—C22—H22	120.1
C35A—C36A—C37A	120.3	C21—C22—H22	120.1
C35A—C36A—H36A	119.9	C22—C23—C24	120.2 (3)
C37A—C36A—H36A	119.9	C22—C23—H23	119.9
C32A—C37A—C36A	119.6	C24—C23—H23	119.9
C32A—C37A—H37A	120.2	C23—C24—C25	120.0 (3)
C36A—C37A—H37A	120.2	C23—C24—H24	120.0
C6—C1—C2	120.57 (19)	C25—C24—H24	120.0
C6—C1—N2	121.49 (18)	C20—C25—C24	120.6 (3)
C2—C1—N2	117.93 (19)	C20—C25—H25	119.7
C3—C2—C1	119.5 (2)	C24—C25—H25	119.7
C3—C2—H2	120.2	C31—C26—C27	118.9 (2)
C1—C2—H2	120.2	C31—C26—Sn1	122.89 (18)
C4—C3—C2	120.6 (2)	C27—C26—Sn1	118.11 (18)
C4—C3—H3	119.7	C28—C27—C26	120.7 (3)
C2—C3—H3	119.7	C28—C27—H27	119.7
C3—C4—C5	119.6 (2)	C26—C27—H27	119.7
C3—C4—H4	120.2	C29—C28—C27	119.3 (3)
C5—C4—H4	120.2	C29—C28—H28	120.3
C6—C5—C4	120.5 (2)	C27—C28—H28	120.3
C6—C5—H5	119.7	C30—C29—C28	121.2 (3)
C4—C5—H5	119.7	C30—C29—H29	119.4
C1—C6—C5	119.2 (2)	C28—C29—H29	119.4
C1—C6—H6	120.4	C29—C30—C31	119.4 (3)
C5—C6—H6	120.4	C29—C30—H30	120.3
N3—C7—H7A	109.5	C31—C30—H30	120.3
N3—C7—H7B	109.5	C26—C31—C30	120.5 (3)
H7A—C7—H7B	109.5	C26—C31—H31	119.7
N3—C7—H7C	109.5	C30—C31—H31	119.7
H7A—C7—H7C	109.5	C12—N1—C10	122.07 (19)
H7B—C7—H7C	109.5	C11—N2—N3	109.44 (16)
C9—C8—H8A	109.5	C11—N2—C1	124.73 (17)
C9—C8—H8B	109.5	N3—N2—C1	120.68 (16)
H8A—C8—H8B	109.5	C9—N3—N2	106.94 (16)
C9—C8—H8C	109.5	C9—N3—C7	124.42 (18)
H8A—C8—H8C	109.5	N2—N3—C7	118.36 (17)
H8B—C8—H8C	109.5	C19—O1—Sn1	117.4 (2)
N3—C9—C10	110.51 (18)	O1—Sn1—C26	111.39 (8)
N3—C9—C8	121.1 (2)	O1—Sn1—C20	107.81 (8)
C10—C9—C8	128.3 (2)	C26—Sn1—C20	116.41 (9)
C9—C10—N1	122.92 (19)	O1—Sn1—C32	91.00 (8)
C9—C10—C11	107.82 (18)	C26—Sn1—C32	110.05 (8)
N1—C10—C11	129.26 (19)	C20—Sn1—C32	117.23 (8)
O3—C11—N2	123.60 (19)	O1—Sn1—C32A	100.30 (7)
O3—C11—C10	131.7 (2)	C26—Sn1—C32A	105.28 (8)
N2—C11—C10	104.70 (17)	C20—Sn1—C32A	114.52 (8)
N1—C12—C13	119.9 (2)	C32—Sn1—C32A	9.4
N1—C12—H12	120.0		

Fig. 1


C35
C34
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C2
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C21
C3
O3
C14
C15
O2
C24
C22
C23

Fig. 2