

Bis(2-fluorobenzyl)(*N*-salicylidene-valinato- κ^3 N,*O*,*O'*)tin(IV)

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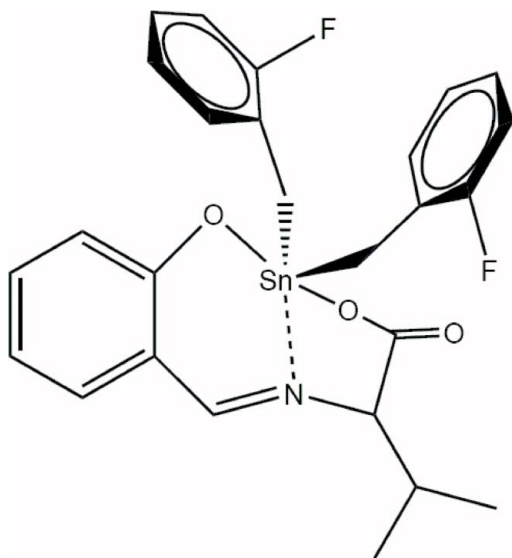
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
Disorder in main residue; R factor = 0.023; wR factor = 0.055; data-to-parameter ratio = 13.1.

In the title compound, $[\text{Sn}(\text{C}_7\text{H}_6\text{F})_2(\text{C}_{12}\text{H}_{13}\text{NO}_3)]$, the Schiff base acts as a tridentate ligand, chelating the Sn atom. The Sn atom is five-coordinate in a distorted trigonal-bipyramidal geometry, with the O atoms occupying the axial positions, and the N and C atoms occupying the equatorial positions. In addition, in the crystal, one of the F atoms is disordered over two positions.

Related literature

Corresponding organotin(IV) complexes with Schiff bases have similar structures (Yin & Wang, 2004; Yin, Wang & Xue, 2004; Beltrán *et al.*, 2003).



Experimental

Crystal data

$[\text{Sn}(\text{C}_7\text{H}_6\text{F})_2(\text{C}_{12}\text{H}_{13}\text{NO}_3)]$
 $M_r = 556.16$
 Triclinic, $P\bar{1}$
 $a = 10.0184$ (16) Å
 $b = 10.5814$ (17) Å
 $c = 11.9367$ (19) Å
 $\alpha = 84.915$ (2)°
 $\beta = 81.776$ (2)°

$\gamma = 68.880$ (2)°
 $V = 1167.3$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.14$ mm⁻¹
 $T = 273$ (2) K
 $0.45 \times 0.41 \times 0.37$ mm

Data collection

Bruker SMART area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
 $T_{\min} = 0.628$, $T_{\max} = 0.678$

6178 measured reflections
 4073 independent reflections
 3698 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.012$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.055$
 $S = 1.12$
 4073 reflections
 310 parameters

1 restraint
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.57$ e Å⁻³
 $\Delta\rho_{\min} = -0.45$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Sn1—O3	2.1104 (17)	Sn1—O1	2.1496 (17)
Sn1—C20	2.140 (3)	Sn1—N1	2.187 (2)
Sn1—C13	2.147 (3)		
O3—Sn1—C20	90.67 (9)	C13—Sn1—O1	97.87 (9)
O3—Sn1—C13	93.05 (9)	O3—Sn1—N1	82.27 (7)
C20—Sn1—C13	129.53 (10)	C20—Sn1—N1	123.25 (9)
O3—Sn1—O1	156.21 (7)	C13—Sn1—N1	107.11 (9)
C20—Sn1—O1	98.42 (9)	O1—Sn1—N1	74.34 (7)

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2289).

References

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supplementary materials

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Bis(2-fluorobenzyl)(*N*-salicylidenevalinato- κ^3 *N,O,O'*)tin(IV)

R. Ding, J. Zhu, D. Zhang, A. Ling and H. Yin

Experimental

A sample of salicylidene-valine (1.0 mmol) and sodium methylate (1.0 mmol) was stirred in 20 ml dichloromethane at room temperature for 30 min. To this solution was added di(*o*-fluorobenzyl)tin dichloride (1.0 mmol). The mixture was stirred at 40°C under nitrogen for 18 h. Evaporation of the filtrate left a yellow solid, which was recrystallized from dichloromethane-hexane (1:3) to give yellow crystals (yield 67%).

Refinement

One of the F atoms is disordered over two positions with site occupation factors of 0.841 (5) and 0.159 (5). All the H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.98 Å and with $U_{\text{iso}}(\text{H}) = 1.2$ (1.5 for methyl groups) times $U_{\text{eq}}(\text{C})$. The methyl groups were allowed to rotate but not to tip.

Figures

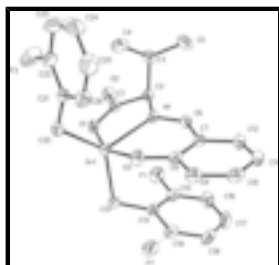


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

(*N*-Salicylidene-valinato-*N,O,O'*) di(*o*-fluorobenzyl)tin(IV)

Crystal data

[Sn(C₁₂H₁₃NO₃)(C₇H₆F)₂]

$M_r = 556.16$

Triclinic, *P* $\bar{1}$

$a = 10.0184$ (16) Å

$b = 10.5814$ (17) Å

$c = 11.9367$ (19) Å

$\alpha = 84.915$ (2)°

$\beta = 81.776$ (2)°

$\gamma = 68.880$ (2)°

$V = 1167.3$ (3) Å³

$Z = 2$

$F_{000} = 560$

$D_x = 1.582$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4740 reflections

$\theta = 2.2$ – 28.0 °

$\mu = 1.14$ mm⁻¹

$T = 273$ (2) K

Block, yellow

$0.45 \times 0.41 \times 0.37$ mm

Data collection

CCD area detector diffractometer	4073 independent reflections
Radiation source: fine-focus sealed tube	3698 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.012$
$T = 273(2)$ K	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -11 \rightarrow 11$
$T_{\text{min}} = 0.628$, $T_{\text{max}} = 0.678$	$k = -12 \rightarrow 9$
6178 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained
$wR(F^2) = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2 + 0.4867P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
4073 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
310 parameters	$\Delta\rho_{\text{max}} = 0.57 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.45 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	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 $F^2 > \sigma(F^2)$ 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn1	0.418762 (18)	0.060765 (17)	0.674028 (14)	0.02904 (7)	
F2	0.1869 (2)	-0.1933 (2)	0.59952 (17)	0.0770 (6)	
N1	0.2350 (2)	0.2516 (2)	0.67652 (16)	0.0302 (5)	
O1	0.37365 (18)	0.10634 (17)	0.50130 (14)	0.0338 (4)	

O2	0.2373 (2)	0.2416 (2)	0.37691 (15)	0.0508 (5)	
O3	0.3804 (2)	0.08235 (18)	0.85103 (14)	0.0387 (4)	
C1	0.2652 (3)	0.2114 (3)	0.4735 (2)	0.0339 (6)	
C2	0.1685 (3)	0.2969 (3)	0.5702 (2)	0.0333 (6)	
H2	0.1605	0.3914	0.5527	0.040*	
C3	0.0169 (3)	0.2891 (3)	0.5788 (2)	0.0407 (7)	
H3	-0.0153	0.3150	0.5037	0.049*	
C4	0.0189 (4)	0.1456 (3)	0.6064 (3)	0.0586 (9)	
H4A	0.0884	0.0853	0.5531	0.088*	
H4B	-0.0748	0.1427	0.6020	0.088*	
H4C	0.0445	0.1181	0.6816	0.088*	
C5	-0.0929 (3)	0.3876 (4)	0.6605 (3)	0.0579 (9)	
H5A	-0.0928	0.4775	0.6410	0.087*	
H5B	-0.0685	0.3624	0.7362	0.087*	
H5C	-0.1868	0.3852	0.6561	0.087*	
C6	0.2016 (3)	0.3394 (3)	0.7549 (2)	0.0349 (6)	
H6	0.1441	0.4272	0.7353	0.042*	
C7	0.2411 (3)	0.3190 (3)	0.8666 (2)	0.0340 (6)	
C8	0.3252 (3)	0.1914 (3)	0.9116 (2)	0.0332 (6)	
C9	0.3474 (3)	0.1824 (3)	1.0263 (2)	0.0428 (7)	
H9	0.4006	0.0994	1.0585	0.051*	
C10	0.2916 (3)	0.2947 (4)	1.0910 (2)	0.0490 (8)	
H10	0.3071	0.2861	1.1668	0.059*	
C11	0.2126 (3)	0.4208 (4)	1.0462 (2)	0.0522 (8)	
H11	0.1771	0.4963	1.0908	0.063*	
C12	0.1881 (3)	0.4322 (3)	0.9360 (2)	0.0459 (7)	
H12	0.1353	0.5165	0.9056	0.055*	
C13	0.6098 (3)	0.1116 (3)	0.6583 (2)	0.0357 (6)	
H13A	0.6837	0.0402	0.6949	0.043*	
H13B	0.6454	0.1171	0.5787	0.043*	
C14	0.5823 (3)	0.2432 (3)	0.7102 (2)	0.0334 (6)	
F1	0.4747 (2)	0.3601 (2)	0.55215 (16)	0.0564 (7)	0.841 (5)
C15	0.51278 (9)	0.3657 (3)	0.65269 (17)	0.0393 (6)	
C19	0.6182 (3)	0.2515 (3)	0.81989 (18)	0.0407 (6)	
H19	0.6646	0.1726	0.8608	0.049*	0.841 (5)
H19'	0.4881	0.3637	0.5808	0.049*	0.159 (5)
F1'	0.6811 (13)	0.1350 (11)	0.8679 (9)	0.058 (4)	0.159 (5)
C16	0.4813 (3)	0.4895 (3)	0.7010 (3)	0.0505 (8)	
H16	0.4366	0.5699	0.6613	0.061*	
C17	0.5164 (4)	0.4930 (3)	0.8075 (3)	0.0544 (8)	
H17	0.4935	0.5758	0.8404	0.065*	
C18	0.5848 (3)	0.3749 (3)	0.8654 (3)	0.0505 (8)	
H18	0.6091	0.3786	0.9371	0.061*	
C20	0.3965 (3)	-0.1340 (3)	0.6949 (2)	0.0365 (6)	
H20A	0.4025	-0.1656	0.6199	0.044*	
H20B	0.4795	-0.1956	0.7291	0.044*	
C21	0.2645 (3)	-0.1481 (2)	0.7631 (2)	0.0336 (6)	
C22	0.1638 (3)	-0.1774 (3)	0.7132 (3)	0.0477 (7)	
C23	0.0419 (4)	-0.1934 (4)	0.7721 (4)	0.0668 (10)	

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H23	-0.0240	-0.2120	0.7348	0.080*
C24	0.0204 (4)	-0.1812 (4)	0.8874 (4)	0.0733 (11)
H24	-0.0615	-0.1904	0.9291	0.088*
C25	0.1196 (4)	-0.1552 (4)	0.9413 (3)	0.0646 (10)
H25	0.1056	-0.1486	1.0196	0.078*
C26	0.2396 (3)	-0.1389 (3)	0.8795 (2)	0.0470 (7)
H26	0.3058	-0.1212	0.9171	0.056*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03388 (10)	0.02846 (10)	0.02714 (10)	-0.01294 (7)	-0.00491 (7)	-0.00292 (7)
F2	0.1004 (16)	0.0969 (16)	0.0589 (12)	-0.0578 (14)	-0.0287 (11)	-0.0034 (11)
N1	0.0316 (11)	0.0329 (12)	0.0252 (10)	-0.0091 (9)	-0.0043 (9)	-0.0053 (9)
O1	0.0366 (10)	0.0330 (10)	0.0274 (9)	-0.0059 (8)	-0.0040 (7)	-0.0061 (7)
O2	0.0570 (13)	0.0585 (13)	0.0241 (10)	-0.0036 (10)	-0.0077 (9)	-0.0027 (9)
O3	0.0546 (12)	0.0358 (10)	0.0259 (9)	-0.0156 (9)	-0.0061 (8)	-0.0022 (8)
C1	0.0361 (14)	0.0371 (15)	0.0271 (13)	-0.0108 (12)	-0.0027 (11)	-0.0048 (11)
C2	0.0373 (14)	0.0328 (14)	0.0261 (12)	-0.0065 (11)	-0.0071 (11)	-0.0023 (11)
C3	0.0355 (15)	0.0496 (17)	0.0335 (14)	-0.0089 (13)	-0.0093 (12)	-0.0016 (13)
C4	0.0514 (19)	0.060 (2)	0.072 (2)	-0.0259 (17)	-0.0119 (17)	-0.0046 (18)
C5	0.0377 (16)	0.068 (2)	0.058 (2)	-0.0084 (15)	0.0013 (14)	-0.0103 (17)
C6	0.0327 (14)	0.0349 (15)	0.0345 (14)	-0.0082 (11)	-0.0031 (11)	-0.0056 (12)
C7	0.0322 (13)	0.0422 (16)	0.0296 (13)	-0.0145 (12)	-0.0005 (11)	-0.0101 (12)
C8	0.0326 (13)	0.0447 (16)	0.0267 (13)	-0.0203 (12)	0.0022 (11)	-0.0044 (12)
C9	0.0449 (16)	0.0571 (19)	0.0278 (13)	-0.0196 (14)	-0.0027 (12)	-0.0046 (13)
C10	0.0444 (17)	0.082 (2)	0.0264 (14)	-0.0270 (17)	-0.0008 (12)	-0.0142 (15)
C11	0.0481 (18)	0.067 (2)	0.0416 (17)	-0.0157 (16)	-0.0012 (14)	-0.0287 (16)
C12	0.0441 (16)	0.0494 (18)	0.0427 (16)	-0.0119 (14)	-0.0030 (13)	-0.0169 (14)
C13	0.0330 (14)	0.0378 (15)	0.0391 (14)	-0.0146 (12)	-0.0035 (11)	-0.0076 (12)
C14	0.0306 (13)	0.0395 (15)	0.0349 (14)	-0.0193 (12)	0.0034 (11)	-0.0085 (12)
F1	0.0777 (16)	0.0574 (14)	0.0390 (12)	-0.0278 (12)	-0.0162 (10)	0.0053 (10)
C15	0.0422 (15)	0.0432 (16)	0.0365 (15)	-0.0204 (13)	-0.0011 (12)	-0.0049 (12)
C19	0.0436 (16)	0.0441 (17)	0.0405 (15)	-0.0220 (13)	-0.0062 (13)	-0.0035 (13)
F1'	0.073 (8)	0.045 (7)	0.057 (7)	-0.014 (6)	-0.035 (6)	0.003 (5)
C16	0.0584 (19)	0.0364 (17)	0.0565 (19)	-0.0200 (14)	0.0024 (15)	-0.0012 (14)
C17	0.066 (2)	0.0431 (18)	0.059 (2)	-0.0264 (16)	0.0089 (16)	-0.0225 (16)
C18	0.062 (2)	0.061 (2)	0.0407 (16)	-0.0347 (17)	-0.0018 (14)	-0.0158 (15)
C20	0.0418 (15)	0.0300 (14)	0.0385 (15)	-0.0142 (12)	-0.0006 (12)	-0.0050 (12)
C21	0.0360 (14)	0.0255 (13)	0.0405 (15)	-0.0125 (11)	-0.0036 (12)	-0.0008 (11)
C22	0.0507 (18)	0.0448 (18)	0.0521 (18)	-0.0200 (14)	-0.0124 (15)	-0.0003 (14)
C23	0.049 (2)	0.062 (2)	0.100 (3)	-0.0296 (17)	-0.020 (2)	0.005 (2)
C24	0.050 (2)	0.069 (2)	0.098 (3)	-0.0284 (19)	0.019 (2)	-0.001 (2)
C25	0.072 (2)	0.070 (2)	0.056 (2)	-0.037 (2)	0.0195 (18)	-0.0093 (18)
C26	0.0517 (18)	0.0477 (18)	0.0452 (17)	-0.0240 (15)	0.0008 (14)	-0.0026 (14)

Geometric parameters (\AA , $^\circ$)

Sn1—O3	2.1104 (17)	C11—H11	0.9300
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Sn1—C20	2.140 (3)	C12—H12	0.9300
Sn1—C13	2.147 (3)	C13—C14	1.493 (4)
Sn1—O1	2.1496 (17)	C13—H13A	0.9700
Sn1—N1	2.187 (2)	C13—H13B	0.9700
F2—C22	1.359 (3)	C14—C15	1.402 (3)
N1—C6	1.300 (3)	C14—C19	1.424 (3)
N1—C2	1.480 (3)	F1—C15	1.323 (3)
O1—C1	1.301 (3)	F1—H19'	0.3947
O2—C1	1.213 (3)	F1'—C19	1.290 (3)
O3—C8	1.316 (3)	F1'—H19	0.378
C1—C2	1.524 (3)	C15—C16	1.390 (4)
C2—C3	1.539 (4)	C15—H19'	0.9300
C2—H2	0.9800	C19—C18	1.368 (4)
C3—C5	1.514 (4)	C19—H19	0.9300
C3—C4	1.519 (4)	C16—C17	1.373 (4)
C3—H3	0.9800	C16—H16	0.9300
C4—H4A	0.9600	C17—C18	1.369 (5)
C4—H4B	0.9600	C17—H17	0.9300
C4—H4C	0.9600	C18—H18	0.9300
C5—H5A	0.9600	C20—C21	1.499 (4)
C5—H5B	0.9600	C20—H20A	0.9700
C5—H5C	0.9600	C20—H20B	0.9700
C6—C7	1.421 (4)	C21—C22	1.378 (4)
C6—H6	0.9300	C21—C26	1.382 (4)
C7—C12	1.412 (4)	C22—C23	1.378 (5)
C7—C8	1.415 (4)	C23—C24	1.372 (5)
C8—C9	1.408 (3)	C23—H23	0.9300
C9—C10	1.372 (4)	C24—C25	1.374 (5)
C9—H9	0.9300	C24—H24	0.9300
C10—C11	1.388 (4)	C25—C26	1.375 (4)
C10—H10	0.9300	C25—H25	0.9300
C11—C12	1.359 (4)	C26—H26	0.9300
O3—Sn1—C20	90.67 (9)	C10—C11—H11	120.5
O3—Sn1—C13	93.05 (9)	C11—C12—C7	121.5 (3)
C20—Sn1—C13	129.53 (10)	C11—C12—H12	119.2
O3—Sn1—O1	156.21 (7)	C7—C12—H12	119.2
C20—Sn1—O1	98.42 (9)	C14—C13—Sn1	111.90 (17)
C13—Sn1—O1	97.87 (9)	C14—C13—H13A	109.2
O3—Sn1—N1	82.27 (7)	Sn1—C13—H13A	109.2
C20—Sn1—N1	123.25 (9)	C14—C13—H13B	109.2
C13—Sn1—N1	107.11 (9)	Sn1—C13—H13B	109.2
O1—Sn1—N1	74.34 (7)	H13A—C13—H13B	107.9
C6—N1—C2	117.7 (2)	C15—C14—C19	117.1 (2)
C6—N1—Sn1	123.80 (17)	C15—C14—C13	120.0 (2)
C2—N1—Sn1	116.80 (15)	C19—C14—C13	122.9 (2)
C1—O1—Sn1	121.60 (15)	C15—F1—H19'	5.1
C8—O3—Sn1	130.98 (16)	F1—C15—C16	120.8 (2)
O2—C1—O1	123.6 (2)	F1—C15—C14	118.1 (2)
O2—C1—C2	119.8 (2)	F1'—C19—C14	113.6 (2)

supplementary materials

O1—C1—C2	116.6 (2)	F1'—C19—C18	126.0 (5)
N1—C2—C1	109.6 (2)	C16—C15—C14	121.1 (2)
N1—C2—C3	112.7 (2)	F1—C15—H19'	2.1
C1—C2—C3	109.5 (2)	F1'—C19—H19	6.2
N1—C2—H2	108.3	C16—C15—H19'	119.7
C1—C2—H2	108.3	C14—C15—H19'	119.2
C3—C2—H2	108.3	C18—C19—C14	120.4 (3)
C5—C3—C4	111.0 (3)	C18—C19—H19	119.8
C5—C3—C2	113.3 (2)	C14—C19—H19	119.8
C4—C3—C2	111.9 (2)	C17—C16—C15	120.0 (3)
C5—C3—H3	106.7	C17—C16—H16	120.0
C4—C3—H3	106.7	C15—C16—H16	120.0
C2—C3—H3	106.7	C18—C17—C16	120.2 (3)
C3—C4—H4A	109.5	C18—C17—H17	119.9
C3—C4—H4B	109.5	C16—C17—H17	119.9
H4A—C4—H4B	109.5	C19—C18—C17	121.3 (3)
C3—C4—H4C	109.5	C19—C18—H18	119.4
H4A—C4—H4C	109.5	C17—C18—H18	119.4
H4B—C4—H4C	109.5	C21—C20—Sn1	119.40 (17)
C3—C5—H5A	109.5	C21—C20—H20A	107.5
C3—C5—H5B	109.5	Sn1—C20—H20A	107.5
H5A—C5—H5B	109.5	C21—C20—H20B	107.5
C3—C5—H5C	109.5	Sn1—C20—H20B	107.5
H5A—C5—H5C	109.5	H20A—C20—H20B	107.0
H5B—C5—H5C	109.5	C22—C21—C26	116.0 (3)
N1—C6—C7	128.7 (2)	C22—C21—C20	121.5 (3)
N1—C6—H6	115.7	C26—C21—C20	122.4 (2)
C7—C6—H6	115.7	F2—C22—C23	118.0 (3)
C12—C7—C8	119.4 (2)	F2—C22—C21	118.2 (3)
C12—C7—C6	117.3 (2)	C23—C22—C21	123.8 (3)
C8—C7—C6	123.3 (2)	C24—C23—C22	118.0 (3)
O3—C8—C9	119.7 (2)	C24—C23—H23	121.0
O3—C8—C7	122.6 (2)	C22—C23—H23	121.0
C9—C8—C7	117.7 (2)	C23—C24—C25	120.2 (3)
C10—C9—C8	120.8 (3)	C23—C24—H24	119.9
C10—C9—H9	119.6	C25—C24—H24	119.9
C8—C9—H9	119.6	C24—C25—C26	120.0 (3)
C9—C10—C11	121.6 (3)	C24—C25—H25	120.0
C9—C10—H10	119.2	C26—C25—H25	120.0
C11—C10—H10	119.2	C25—C26—C21	121.8 (3)
C12—C11—C10	119.0 (3)	C25—C26—H26	119.1
C12—C11—H11	120.5	C21—C26—H26	119.1

Fig. 1

