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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 = 0.030
 wR factor = 0.079
Data-to-parameter ratio = 22.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3-Methoxy-*N*-[2-(methylsulfonyl)phenyl]-
salicylaldimineThe molecule of the title compound, $\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$, is nearly planar, with a dihedral angle of 6.78 (7)° between the benzene rings. The planarity of the molecule is promoted by an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond.

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Comment

Schiff base ligands are common in coordination chemistry (Che & Huang, 2003). Our group is interested in the synthesis and coordination chemistry of novel sulfur-containing mixed-donor ligands (Hamaker & Halbach, 2006). As part of these ongoing studies, we report here the synthesis and crystal structure of the title compound, (I).

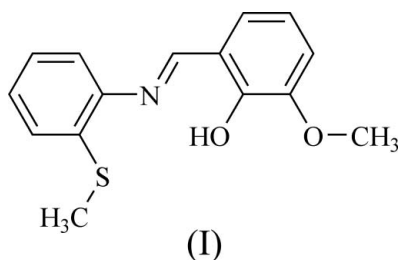
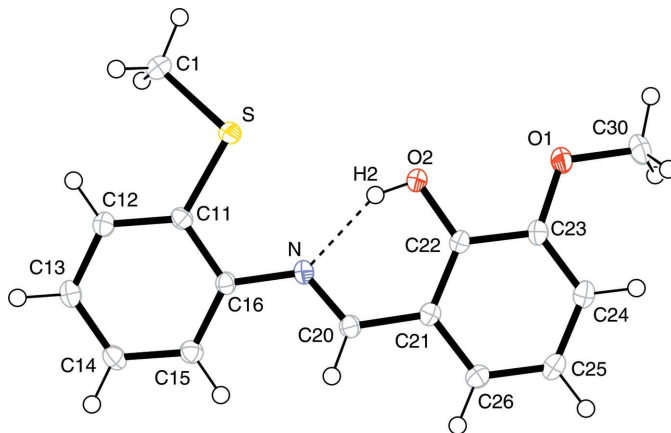
The molecule of compound (I) (Fig. 1) is nearly planar, with a dihedral angle between the two aromatic rings of 6.78 (7)° and a $\text{C}21-\text{C}20-\text{N}-\text{C}16$ torsion angle of 179.07 (11)°. The planarity of (I) is promoted by an intramolecular $\text{O}2-\text{H}2\cdots\text{N}$ hydrogen bond (Table 2). The bond lengths and angles (Table 1) are similar to those of related Schiff base compounds (Singh *et al.*, 2004; Yeap *et al.*, 2003; Francis *et al.*, 2003).

Figure 1

A view of (I), showing the atom-numbering scheme and with 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

Experimental

To a solution of 2-(methylthio)aniline (2.778 g, 19.95 mmol) in absolute ethanol (50 ml) in a 100 ml round-bottomed flask equipped with a reflux condenser, *o*-vanillin was added (3.061 g, 20.12 mmol). The mixture was heated to reflux for 1.5 h, cooled to room temperature and placed in a freezer at 233 K for 14 h. The reaction product was filtered off, washed with cold ethanol and dried *in vacuo* to yield 4.700 g (86%) of the title compound as an orange solid. Crystals of (I) were grown by slow evaporation of an ethanol solution (m.p. 384–386 K). Spectroscopic analysis: ^1H NMR (CDCl_3 , 400 MHz, δ , p.p.m.): 13.35 (s, 1H, OH), 8.65 (s, 1H, N=CH), 7.27 (m, 2H, arom.), 7.21 (m, 2H, arom.), 7.05 (dd, 1H, arom.), 7.01 (dd, 1H, arom.), 6.89 (t, 1H, arom.), 3.90 (s, 3H, OCH_3), 2.48 (s, 3H, SCH_3); ^{13}C NMR (CDCl_3 , 400 MHz, δ , p.p.m.): 162.4, 151.9, 149.0, 145.6, 135.5, 128.0, 125.8, 125.6, 124.4, 119.8, 119.0, 117.6, 115.9, 56.7, 15.3; IR (Nujol, ν , cm^{-1}): 1610 (C=N); UV-vis (CH_2Cl_2): λ_{max} (ϵ) 361 nm ($8230 \text{ M}^{-1} \text{ cm}^{-1}$), 273 nm ($19\,100 \text{ M}^{-1} \text{ cm}^{-1}$). Analysis calculated (found) for $\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$: C 65.91 (65.76), H 5.53 (5.46), N 5.12 (5.17)%.

Crystal data

$\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$	Mo $K\alpha$ radiation
$M_r = 273.34$	Cell parameters from 7027 reflections
Orthorhombic, $Pca2_1$	$\theta = 3.0\text{--}30.5^\circ$
$a = 6.5559$ (4) Å	$\mu = 0.25 \text{ mm}^{-1}$
$b = 13.7147$ (7) Å	$T = 100$ (2) K
$c = 14.5200$ (8) Å	Block, orange-yellow
$V = 1305.53$ (13) Å ³	$0.59 \times 0.33 \times 0.32 \text{ mm}$
$Z = 4$	
$D_x = 1.391 \text{ Mg m}^{-3}$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3900 independent reflections
φ and ω scans	3875 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2003)	$R_{\text{int}} = 0.020$
$T_{\text{min}} = 0.841$, $T_{\text{max}} = 0.930$	$\theta_{\text{max}} = 30.5^\circ$
14274 measured reflections	$h = -9 \rightarrow 9$
	$k = -19 \rightarrow 19$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.4174P]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.079$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.13$	$\Delta\rho_{\text{max}} = 0.30 \text{ e } \text{Å}^{-3}$
3900 reflections	$\Delta\rho_{\text{min}} = -0.22 \text{ e } \text{Å}^{-3}$
176 parameters	Absolute structure: Flack (1983),
H atoms treated by a mixture of independent and constrained refinement	with 1831 Friedel pairs
	Flack parameter: 0.06 (5)

Table 1

Selected geometric parameters (Å, °).

C16–N	1.4150 (16)	C20–N	1.2868 (16)
N–C20–C21	121.69 (11)	C20–N–C16	122.44 (11)

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$\text{O2--H2}\cdots\text{N}$	0.79 (2)	1.90 (3)	2.6255 (15)	152 (2)

The H atom of the hydroxyl group was found in a difference Fourier map and refined isotropically. The other H atoms were treated as riding atoms, with C–H distances of 0.95 Å (aromatic) or 0.98 Å (aliphatic), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the aromatic and CH_2 H atoms or $1.5U_{\text{eq}}(\text{C})$ for the CH_3 H atoms.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SIR2002 (Burla *et al.*, 2003); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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