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4-Bromo-2-formyl-6-methoxyphenyl benzenesulfonate

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Key indicators

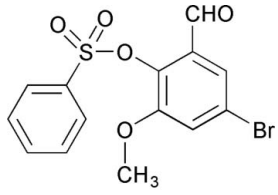
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.086
Data-to-parameter ratio = 15.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{14}H_{11}BrO_5S$, the *o*-vanillin group makes a dihedral angle of 44.96 (8)° with the phenyl ring. Molecules form centrosymmetric dimers *via* C—H···O hydrogen bonds; short Br···O contacts are present between dimers.

Comment

Schiff base ligands have received a good deal of attention in biology and chemistry (Kahwa *et al.*, 1986). Many Schiff base derivatives have been synthesized and employed in the development of protein and enzyme mimics (Santos *et al.*, 2001). As a part of our interest in the coordination properties of Schiff bases functioning as ligands, we have investigated the title compound, (I), which is used as a precursor in the preparation of Schiff bases.



(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The *o*-vanillin group (atoms C7–C13/O3/O4) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.018Å, and makes a dihedral angle of 44.96 (8)° with the phenyl ring (C1–C6). Molecules of (I) form centrosym-

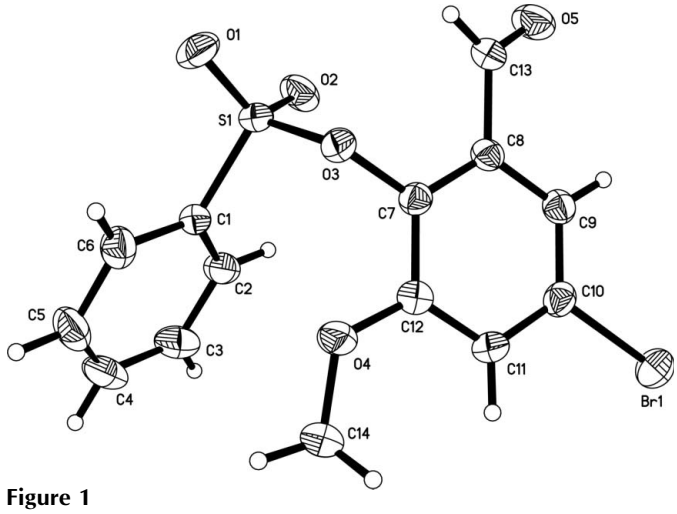


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level for non-H atoms.

metric dimers through C6—H6···O4^{i} hydrogen bonds (symmetry code as in Table 1; Fig. 2). Short Br1···O2^{ii} (symmetry code: (ii) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$) contacts of 3.275 (2) Å are present between dimers.

Experimental

An anhydrous benzene solution (100 ml) of 5-bromo-2-hydroxy-3-methoxybenzaldehyde (2.31 g, 10 mmol) was added dropwise over 30 min to a solution (50 ml) of benzenesulfonyl chloride (1.76 g, 10 mmol) and pyridine (0.79 g, 10 mmol) in benzene, and the mixture was refluxed for 24 h under a nitrogen atmosphere. The solvent was removed and the resulting mixture poured into ice–water (100 ml). The resulting white precipitate was isolated, recrystallized from acetonitrile and dried in a vacuum to give the pure compound in 65% yield. Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{14}H_{11}BrO_5S$
$M_r = 371.20$
Monoclinic, $P2_1/c$
$a = 7.886$ (3) Å
$b = 22.445$ (9) Å
$c = 8.268$ (3) Å
$\beta = 97.019$ (7)°
$V = 1452.5$ (10) Å^3
$Z = 4$
$D_x = 1.697$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.99$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.38 × 0.24 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.411$, $T_{max} = 0.584$
7939 measured reflections
2884 independent reflections
2190 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 26.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.086$
$S = 1.02$
2884 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.6897P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O4^{i}	0.93	2.62	3.436 (4)	148

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

H atoms were included in calculated positions and refined using a riding model, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for Csp^2, or C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3. The methyl group was allowed to rotate about its local threefold axis.

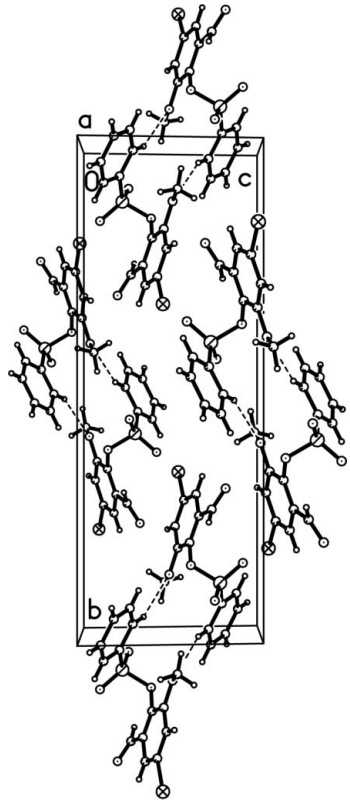


Figure 2
Perspective view of (I) along *a*, showing molecules linked into centrosymmetric dimers by C—H···O interactions (dashed lines).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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