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(*E*)-2-Methoxy-*N*′-[3-(4-methylphenylsulfonyloxy)-benzylidene]benzohydrazide acetic acid solvate

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Key indicators

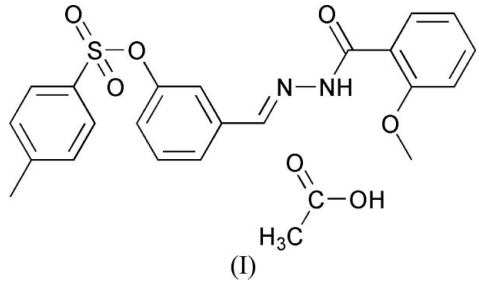
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.154
Data-to-parameter ratio = 13.3

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

In the title compound, $C_{22}H_{20}N_2O_5S\cdot C_2H_4O_2$, the central benzene ring makes dihedral angles of 55.41 (9) and 3.88 (14)° with the two other benzene rings. An intramolecular N—H···O hydrogen bond helps to stabilize the molecular conformation, while intermolecular O—H···O and C—H···O hydrogen bonds link adjacent molecules to form an infinite network.

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 to develop protein and enzyme mimics (Santos *et al.*, 2001), such as models to mimic hydrolase in the hydrolysis of *p*-nitrophenyl picolinate (Li *et al.*, 2005). Structural information is useful when investigating the coordination properties of Schiff bases functioning as ligands. We report here the synthesis and molecular structure of the title Schiff base compound, (I) (Fig. 1).



(I)

In (I), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The central benzene ring (atoms C8–C14/O3) makes dihedral angles of 55.41 (9) and 3.88 (14)°, respectively, with the C1–C6 and C16–C21 benzene rings, while the dihedral angle between these two benzene rings is 59.15 (10)°.

An intramolecular hydrogen bond links the NH group to atom O5, thereby influencing the molecular conformation. There is also an O—H···O intermolecular hydrogen bond linking the main molecule and the solvent molecule. The crystal structure is stabilized by three weak non-classical intermolecular C—H···O hydrogen bonds (Table 1), forming an infinite network (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 3-formylphenyl-4-methylbenzenesulfonic acid (2.76 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 2-methoxybenzohydrazide (1.66 g,

10 mmol) and the mixture stirred at 350 K for 3 h under N_2, giving a white precipitate. The product was isolated, recrystallized from ethanol, and then dried in a vacuum to give pure compound (I) in 85% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol–acetic acid (1:1) solution.

Crystal data

$C_{22}H_{20}N_2O_5S\cdot C_2H_4O_2$
M_r = 484.52
Triclinic, $P\overline{1}$
a = 8.2869 (15) Å
b = 8.9350 (16) Å
c = 16.375 (3) Å
α = 92.368 (3)°
β = 102.547 (3)°
γ = 95.484 (3)°
V = 1175.7 (4) Å^3
Z = 2
D_x = 1.369 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 294 (2) K
Block, colorless
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.938, T_{max} = 0.964
6010 measured reflections
4118 independent reflections
3137 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.154
S = 1.07
4118 reflections
310 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0825P)^2 + 0.3853P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O5	0.86	1.93	2.616 (3)	135
O6—H6A···O4^{i}	0.82	2.06	2.709 (3)	136
C10—H10···O1^{i}	0.93	2.49	3.239 (3)	137
C6—H6···O1^{ii}	0.93	2.56	3.382 (4)	148
C7—H7A···O1^{iii}	0.96	2.54	3.460 (4)	160

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y, -z+1$; (iii) $-x, -y, -z+1$.

The H atoms were included in calculated positions and refined using a riding-model approximation. Constrained C—H and N—H bond lengths and isotropic U_{iso}(H) parameters: 0.93 Å and 1.2U_{eq}(C) for Csp^2, 0.96 Å and 1.5U_{eq}(C) for methyl, and 0.86 Å and 1.2U_{eq}(N) for imino H atoms.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

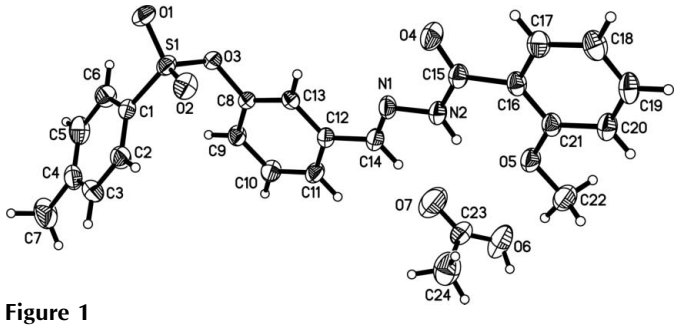


Figure 1
The molecular structure of (I), showing the atom-labeling scheme, with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

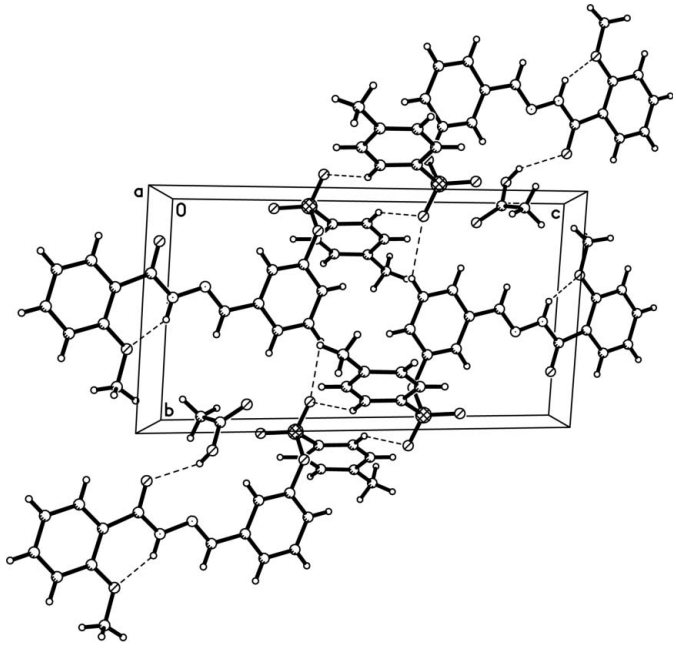


Figure 2
A packing diagram for (I), with hydrogen bonds shown as dashed lines.

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