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Key indicators

Single-crystal X-ray study T = 298 KMean $\sigma(\text{C-C}) = 0.003 \text{ Å}$ R factor = 0.035 wR factor = 0.102Data-to-parameter ratio = 10.3

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

(*E*)-2-Hydroxy-*N*′-[1-(4-methoxyphenyl)-ethylidene]benzohydrazide

The title molecule, $C_{16}H_{16}N_2O_3$, adopts a *trans* configuration with respect to the C \equiv N double bond. The dihedral angle between the two rings is 47.2 (3)°. The crystal structure is stabilized by intermolecular $O-H\cdots O$ hydrogen bonds, which link the molecules into a chain parallel to the *b* axis.

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Comment

Recently, we have reported several Schiff base complexes (Qiu, Yang et al., 2006; Qiu, Ma et al., 2006). As an extension of our work on the structural characterization of Schiff base compounds, the title compound, (I), is reported here (Fig. 1).

In the title compound, (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The C8=N2 bond length of 1.277 (3) Å conforms to the value for a double bond, while the C7-N1 bond [1.337 (2) Å] is greater than the value for a double bond and less than the value for a single bond because of conjugation effects in the molecule. The dihedral angle between the benzene rings is 47.2 (3)°.

In the crystal structure, the molecules are linked through weak intermolecular $N-H\cdots O$ and $O-H\cdots O$ hydrogen bonds, forming a chain parallel to the b axis (Table 1 and Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. 1-(4-Methoxyphenyl)ethanone (0.1 mmol,

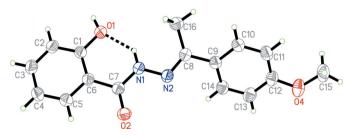


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates an intramolecular hydrogen bond.

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15.0 mg) and 2-hydroxybenzohydrazide (0.1 mmol, 15.1 mg) were dissolved in ethyl acetate (15 ml). The reaction mixture was heated at 393 K for 3 h with stirring. A white solid precipitated from the solution; this was dissolved in acetone (12 ml) and stirred for about 10 min to give a clear colourless solution. After allowing the solution to stand in air for 8 d, colourless block-shaped crystals formed at the bottom of the vesssl on slow evoporation of the solvent. They were collected, washed three times with acetone and dried in a vacuum desiccator using CaCl₂. The compound was isolated in 53% yield.

Crystal data

$C_{16}H_{16}N_2O_3$	Z = 4		
$M_r = 284.31$	$D_x = 1.328 \text{ Mg m}^{-3}$		
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation		
a = 7.4007 (15) Å	$\mu = 0.09 \text{ mm}^{-1}$		
b = 11.794 (2) Å	T = 298 (2) K		
c = 16.290 (3) Å	Block, colourless		
$V = 1421.8 (5) \text{ Å}^3$	$0.26 \times 0.12 \times 0.07 \text{ mm}$		

Data collection

Bruker SMART APEX area-	10760 measured reflections
detector diffractometer	1992 independent reflections
ω scans	1341 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan	$R_{\rm int} = 0.030$
(SADABS; Sheldrick, 1996)	$\theta_{ m max} = 28.2^{\circ}$
$T_{\min} = 0.984, T_{\max} = 0.991$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_0^2) + (0.0368P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	+ 0.1085P
$wR(F^2) = 0.102$	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{\rm max} < 0.001$
1992 reflections	$\Delta \rho_{\text{max}} = 0.12 \text{ e Å}^{-3}$
193 parameters	$\Delta \rho_{\min} = -0.12 \text{ e Å}^{-3}$
H-atom parameters constrained	Extinction correction: SHELXL97
	Extinction coefficient: 0.008 (2)

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

$D-H\cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	$D-H\cdots A$
$ \begin{array}{c} N1-H1\cdots O1 \\ O1-H1A\cdots O2^{i} \end{array} $	0.86	1.93	2.603 (2)	134
	0.82	1.77	2.573 (2)	168

Symmetry code: (i) -x + 2, $y - \frac{1}{2}$, $-z + \frac{1}{2}$.

All H atoms were placed in geometrically idealized positions (O– H = 0.82 Å, N–H = 0.86 Å and C–H = 0.93 or 0.96 Å) and constrained to ride on their parent atoms. They were treated as riding

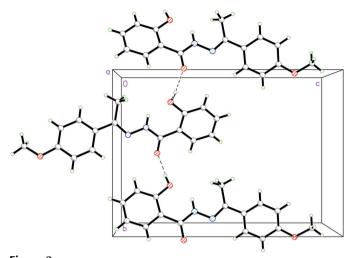


Figure 2
The crystal packing of (I). Dashed lines indicate intermolecular hydrogen bonds.

atoms; $U_{\rm iso}({\rm H})=1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}({\rm methyl~C,O})$. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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