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## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=298 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.003 \AA$
$R$ factor $=0.035$
$w R$ factor $=0.102$
Data-to-parameter ratio $=10.3$

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

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## (E)-2-Hydroxy- $\mathrm{N}^{\prime}$-[1-(4-methoxyphenyl)ethylidene]benzohydrazide

The title molecule, $\mathrm{C}_{16} \mathrm{H}_{16} \mathrm{~N}_{2} \mathrm{O}_{3}$, adopts a trans configuration with respect to the $\mathrm{C}=\mathrm{N}$ double bond. The dihedral angle between the two rings is $47.2(3)^{\circ}$. The crystal structure is stabilized by intermolecular $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds, which link the molecules into a chain parallel to the $b$ axis.

## 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 $\mathrm{C} 8=\mathrm{N} 2$ bond length of 1.277 (3) $\AA$ conforms to the value for a double bond, while the $\mathrm{C} 7-\mathrm{N} 1$ bond $[1.337$ (2) $\AA$ ] 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 $47.2(3)^{\circ}$.

In the crystal structure, the molecules are linked through weak intermolecular $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}$ and $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ 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 $(0.1 \mathrm{mmol}$,


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 ( $0.1 \mathrm{mmol}, 15.1 \mathrm{mg}$ ) were dissolved in ethyl acetate $(15 \mathrm{ml})$. 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 $\mathrm{CaCl}_{2}$. The compound was isolated in $53 \%$ yield.

## Crystal data

$\mathrm{C}_{16} \mathrm{H}_{16} \mathrm{~N}_{2} \mathrm{O}_{3}$
$M_{r}=284.31$
Orthorhombic, $P_{2} 2_{1} 2_{1} 2_{1}$
$a=7.4007(15) \AA$
$b=11.794(2) \AA$
$c=16.290(3) \AA$
$V=1421.8(5) \AA$

$$
\begin{aligned}
& Z=4 \\
& D_{x}=1.328 \mathrm{Mg} \mathrm{~m}^{-3} \\
& \text { Mo } K \alpha \text { radiation } \\
& \mu=0.09 \mathrm{~mm}^{-1} \\
& T=298(2) \mathrm{K} \\
& \text { Block, colourless } \\
& 0.26 \times 0.12 \times 0.07 \mathrm{~mm}
\end{aligned}
$$

## Data collection

Bruker SMART APEX areadetector diffractometer

## $\omega$ scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{\text {min }}=0.984, T_{\text {max }}=0.991$

## Refinement

Refinement on $F^{2}$
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.035$
$w R\left(F^{2}\right)=0.102$
$S=1.03$
1992 reflections
193 parameters
H -atom parameters constrained

10760 measured reflections 1992 independent reflections 1341 reflections with $I>2 \sigma(I)$ $R_{\text {int }}=0.030$ $\theta_{\text {max }}=28.2^{\circ}$

$$
\begin{aligned}
& w= 1 /\left[\sigma^{2}\left(F_{\mathrm{o}}^{2}\right)+(0.0368 P)^{2}\right. \\
&+0.1085 P] \\
& \text { where } P=\left(F_{\mathrm{o}}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3 \\
&(\Delta / \sigma)_{\max }<0.001 \\
& \Delta \rho_{\max }=0.12 \mathrm{e} \AA^{-3} \\
& \Delta \rho_{\min }=-0.12 \mathrm{e}^{-3}
\end{aligned}
$$

Extinction correction: SHELXL97
Extinction coefficient: 0.008 (2)

Table 1
Hydrogen-bond geometry ( $\mathrm{A}^{\circ},{ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| N1-H1 $\cdots$ O1 | 0.86 | 1.93 | $2.603(2)$ | 134 |
| O1-H1 $\cdots$ O $^{\mathrm{i}}$ | 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 ( $\mathrm{O}-$ $\mathrm{H}=0.82 \AA, \mathrm{~N}-\mathrm{H}=0.86 \AA$ and $\mathrm{C}-\mathrm{H}=0.93$ or $0.96 \AA$ ) 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; $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C})$ or $1.5 U_{\text {eq }}$ (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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