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## Structure Reports

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## Nurziana Ngah, Nuriah Mohamad, Musa Ahmad and Bohari M. Yamin*

School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

Correspondence e-mail:
bohari@pkrisc.cc.ukm.my

## Key indicators

Single-crystal X-ray study
$T=273 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.003 \AA$
$R$ factor $=0.059$
$w R$ factor $=0.138$
Data-to-parameter ratio $=14.8$
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.
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## 1-(2-Hydroxyphenyl)ethanone benzoylhydrazone

In the title compound, the planes of the phenyl and 2-(1iminoethyl)phenol fragments form dihedral angles of 28.18 (11) and $28.51(11)^{\circ}$, respectively, with the central $-\mathrm{N}-\mathrm{C}(=\mathrm{O})-$ fragment. The molecule is stabilized by intermolecular $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds, which form a onedimensional chain parallel to the $a$ axis.

## Comment

The title compound, (I), is the product of the condensation reaction of benzhydrazide with 2-hydroxyacetophenone. Like many benzoylhydrazone derivatives, the molecule exists in the keto tautomeric form (Fig. 1).

(I)

The phenyl (C1-C6), 2-(1-imino-ethyl)phenol (C10-C15/ $\mathrm{O} 2 / \mathrm{C} 8 / \mathrm{C} 9 / \mathrm{N} 2$ ) and $\mathrm{N} 1 / \mathrm{C} 7 / \mathrm{O} 1$ framents are each planar, with maximum deviations of 0.011 (2) $\AA$ for atoms C3 and C6. The geometric parameters of the molecule are in normal ranges (Allen et al., 1987) and in agreement with other benzoylhydrazone compounds, such as 1-(4-fluoro-2-hydroxyphenyl)ethanone 4-nitrobenzoylhydrazone (Ali et al., 2004).

The molecule of (I) resembles an asymmetric wing. The planes of the phenyl and 2-(1-imino-ethyl)phenol fragments form dihedral angles of 28.18 (11) and $28.51(11)^{\circ}$, respectively, with the central $\mathrm{N} 1 / \mathrm{C} 7 / \mathrm{O} 1$ fragment. The dihedral angle


Figure 1
The molecular structure of (I), with the atom-numbering scheme and $50 \%$ probability displacement ellipsoids.
between the phenyl and 2-(1-imino-ethyl)phenol groups is 11.15 (10) ${ }^{\circ}$.

There are two intramolecular $\mathrm{O} 2-\mathrm{H} 2 A \cdots \mathrm{~N} 2$ and $\mathrm{C} 9-$ $\mathrm{H} 9 A \cdots \mathrm{~N} 1$ hydrogen bonds. In the crystal structure, the molecules are stabilized by intermolecular $\mathrm{N} 1-\mathrm{H} 1 B \cdots \mathrm{O} 1^{1}$ hydrogen bonds (symmetry code given in Table 2) to form a one-dimensional chain parallel to the $a$ axis (Fig. 2).

## Experimental

An equimolar mixture of benzhydrazide ( 10 mmol ) and 2-hydroxyphenylacetophenone ( 10 mmol ) in ethanol was refluxed in a twonecked round-bottomed flask for 2 h . The solution was then filtered to remove some undissolved solids. Colourless crystals of (I) were obtained in the filtrate after 1 h of evaporation at room temperature (yield $90 \%$; m.p. $446-447 \mathrm{~K}$ ). Analysis, calculated: C 70.84, H 5.55, N 11.02 , O $12.59 \%$; found: C 69.92 , H 5.60 , N 11.00 , O $12.38 \%$.

## Crystal data

$\mathrm{C}_{15} \mathrm{H}_{14} \mathrm{~N}_{2} \mathrm{O}_{2}$
$M_{r}=254.28$
Monoclinic, $P 2_{1} / n$
$a=4.9110(18) \AA$
$b=12.466(4) \AA$
$c=21.018(7) \AA$
$\beta=91.299(6)$
$V=1286.4(8) \AA^{\circ}$
$Z=4$

$$
D_{x}=1.313 \mathrm{Mg} \mathrm{~m}^{-3}
$$

$M_{r}=254.28$
Monoclinic, $P 2_{1} / n$
$b=12.466$ (4) $\AA$
$c=21.018$ (7) A
$V=1286.4(8) \AA^{3}$
$Z=4$
Mo $K \alpha$ radiation
Cell parameters from 1000 reflections
$\theta=1.9-26.5^{\circ}$
$\mu=0.09 \mathrm{~mm}^{-1}$
$T=273$ (2) K
Block, colourless
$0.43 \times 0.22 \times 0.19 \mathrm{~mm}$

## Data collection

| Bruker SMART APEX CCD area- | 2662 independent reflections |
| :--- | :--- |
| detector diffractometer | 2342 reflections with $I>2 \sigma(I)$ |
| $\omega$ scans | $R_{\text {int }}=0.030$ |
| Absorption correction: multi-scan | $\theta_{\max }=26.5^{\circ}$ |
| $\quad(S A D A B S ;$ Sheldrick, 1996$)$ | $h=-6 \rightarrow 6$ |
| $T_{\min }=0.964, T_{\max }=0.985$ | $k=-15 \rightarrow 15$ |
| 13472 measured reflections | $l=-26 \rightarrow 26$ |

## Refinement

Refinement on $F^{2}$
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.059$
$w R\left(F^{2}\right)=0.138$
$S=1.24$
2662 reflections
180 parameters
H atoms treated by a mixture of independent and constrained refinement

$$
\begin{aligned}
& w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}{ }^{2}\right)+(0.0477 P)^{2}\right. \\
& +0.3287 P] \\
& \text { where } P=\left(F_{\mathrm{o}}{ }^{2}+2{F_{\mathrm{c}}}^{2}\right) / 3 \\
& (\Delta / \sigma)_{\max }<0.001 \\
& \Delta \rho_{\max }=0.15 \mathrm{e}_{\AA^{-3}} \\
& \Delta \rho_{\min }=-0.13 \mathrm{e}^{-3} \\
& \text { Extinction correction: none }
\end{aligned}
$$

Table 1
Selected geometric parameters ( $\left({ }^{\circ},{ }^{\circ}\right)$.

| O1-C7 | $1.227(2)$ | $\mathrm{N} 2-\mathrm{N} 1$ | $1.387(2)$ |
| :--- | :---: | :--- | ---: |
| $\mathrm{N} 2-\mathrm{C} 8$ | $1.285(2)$ | $\mathrm{C} 7-\mathrm{N} 1$ | $1.350(2)$ |
|  |  |  |  |
| C1-C6-C7-O1 | $150.85(18)$ | $\mathrm{C} 8-\mathrm{N} 2-\mathrm{N} 1-\mathrm{C} 7$ | $-158.92(16)$ |
| $\mathrm{O} 1-\mathrm{C} 7-\mathrm{N} 1-\mathrm{N} 2$ | $10.0(3)$ |  |  |



Figure 2
A packing diagram for (I), viewed down the $b$ axis. Dashed lines denote $\mathrm{N} 1-\mathrm{H} 1 B \cdots \mathrm{O} 1$ hydrogen bonds.

Table 2
Hydrogen-bond geometry ( $\AA^{\circ},{ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{O} 2-\mathrm{H} 2 A \cdots \mathrm{~N} 2$ | $0.82(3)$ | $1.81(3)$ | $2.545(2)$ | $148(3)$ |
| $\mathrm{C} 9-\mathrm{H} 9 A \cdots \mathrm{~N} 1$ | 0.96 | 2.36 | $2.792(3)$ | 107 |
| $\mathrm{~N} 1-\mathrm{H} 1 B \cdots \mathrm{O}^{\mathrm{i}}$ | $0.83(2)$ | $2.10(2)$ | $2.919(2)$ | $165(2)$ |

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

All H atoms were located in a difference map. Atoms H1B and $\mathrm{H} 2 A$ were refined isotropically. All other H atoms were positioned geometrically and allowed to ride on their parent C atoms, with $\mathrm{C}-\mathrm{H}$ distances in the range $0.93-0.96 \AA$, and with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C})$ for CH and $1.5_{\mathrm{eq}}(\mathrm{C})$ for $\mathrm{CH}_{3}$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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