

Fu-You Pan* and Jian-Guo Yang

Department of Chemistry, Taizhou University,
 Taizhou 317000, People's Republic of China

Correspondence e-mail: panfy@tzc.edu.cn

Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C)$ = 0.006 Å
 R factor = 0.044
 wR factor = 0.140
 Data-to-parameter ratio = 12.3

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

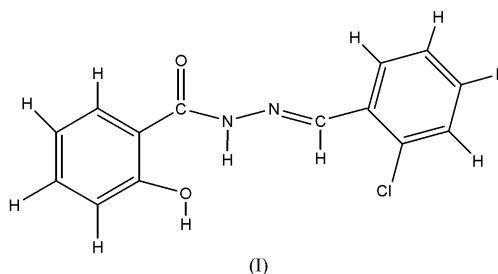
**N'-(2-Chlorobenzylidene)-2-hydroxybenzo-
 hydrazide**

The title compound, C₁₄H₁₁ClN₂O₂, was synthesized by the reaction of 2-hydroxybenzoylhydrazine with 2-chlorobenzaldehyde in ethanol. The crystal structure involves intermolecular O—H···O and intramolecular N—H···O hydrogen bonds.

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Comment

Some benzoylhydrazone compounds possess bacteriostatic activity. This type of compound has wide application in tuberculosis treatment and also exhibits fungicidal activity (Edwards *et al.*, 1975). Furthermore, the hydrazonecarbonyl is a structural motif showing bioactivity (Zhi *et al.*, 2003; Yang & Pan, 2004). In order to search for more effective antibacterial medicines, we have synthesized the title compound, (I).



Due to conjugation, the C=O distance [1.218 (4) Å] is longer than the normal value of 1.20 Å, while C8—N2 [1.351 (5) Å] is longer than the C=N bond distance (1.32 Å; John, 1998) and shorter than the C—N single-bond distance (1.475 Å; John, 1998). An intermolecular O—H···O hydrogen bond is observed, linking the hydroxyl H atom with the carbonyl group of an adjacent molecule. In addition, there is an intramolecular N—H···O hydrogen bond between the amide NH and hydroxyl groups, forming a six-membered ring (Fig. 2). Symmetry-related molecules are linked along the *c*

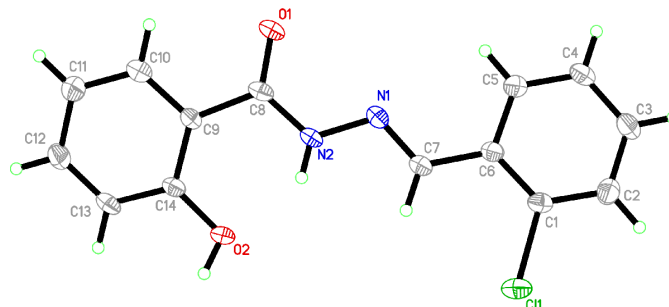


Figure 1
 The structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

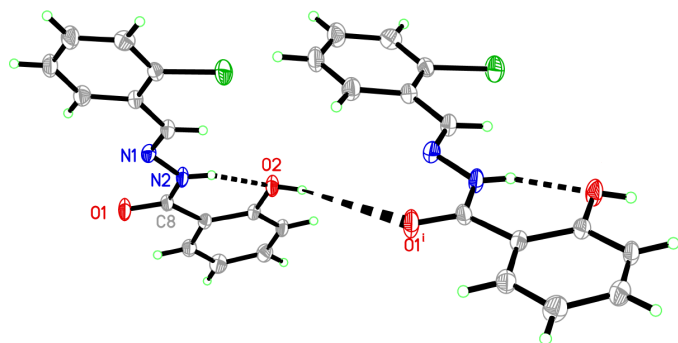


Figure 2
Two molecules of (I), showing the inter- and intramolecular hydrogen bonds as dashed lines [symmetry code (i): $x, -y + \frac{1}{2}, z + \frac{1}{2}$].

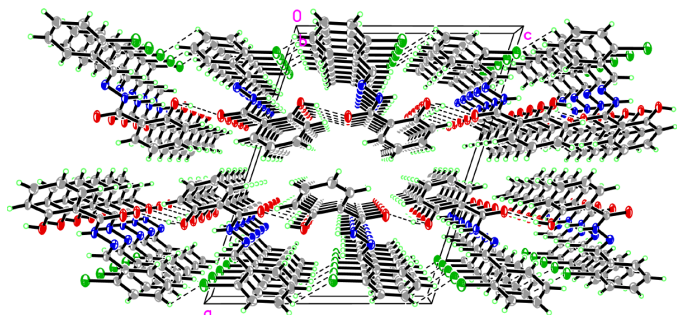


Figure 3
The packing of (I), viewed down the b axis, showing the hydrogen-bonded (dashed lines) chains.

direction via $O-H \cdots O$ hydrogen bonds to form a chain (Fig. 3).

Experimental

2-Hydroxybenzoylhydrazine (0.02 mol, 3.04 g) was dissolved in anhydrous ethanol (50 ml) at room temperature. 2-Chlorobenzaldehyde (0.02 mol, 2.81 g) was added and the mixture was refluxed for 2 h. The precipitate was collected by filtration and washed with ethanol. The product was recrystallized from ethanol and dried under reduced pressure to give the title compound. The compound (2.0 mmol, 0.55 g) was dissolved in dimethylformamide (30 ml) and kept at room temperature for 30 d, after which time colourless parallelepiped single crystals had formed, and these were collected and washed with distilled water.

Crystal data

$C_{14}H_{11}ClN_2O_2$
 $M_r = 274.70$
Monoclinic, $P2_1/c$
 $a = 16.884$ (3) Å
 $b = 5.873$ (2) Å
 $c = 13.135$ (3) Å
 $\beta = 108.38$ (1)°
 $V = 1236.0$ (6) Å³
 $Z = 4$

$D_x = 1.476$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
 $\theta = 8.8$ – 11.7 °
 $\mu = 0.31$ mm⁻¹
 $T = 295$ (2) K
Parallelepiped, colourless
 $0.20 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.941, T_{\max} = 0.970$
2507 measured reflections

2209 independent reflections
919 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$
 $\theta_{\max} = 25.2$ °
 $h = -19 \rightarrow 20$
 $k = -7 \rightarrow 0$
 $l = -15 \rightarrow 1$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.140$
 $S = 0.98$
2209 reflections
180 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 0.0065P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.34$ e Å⁻³

Table 1

Selected bond lengths (Å).

O1—C8	1.218 (4)	N2—C8	1.351 (5)
O2—C14	1.362 (5)		

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H1 \cdots O2	0.81 (3)	1.98 (4)	2.646 (4)	139 (4)
O2—H6 \cdots O1 ⁱ	0.84 (6)	1.87 (6)	2.663 (4)	159 (6)

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

All H atoms, except H1 and H6, were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å (C—H). Atoms H1 and H6 were located in a difference Fourier map and their parameters were refined.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); 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, 2002); software used to prepare material for publication: SHELXTL.

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References

- Bruker (2002). SMART, SAINT, SADABS and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
Edwards, E. I., Epton, R. & Marr, G. (1975). *J. Organomet. Chem.* **85**, C23–C25.
John, A. D. (1998). *Lange's Handbook of Chemistry*, Vol. 4, pp. 39–41. Beijing: Science Publishing Company.
Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
Yang, J. G. & Pan, F. Y. (2004). *Acta Cryst.* **E60**, o2009–o2010.
Zhi, J. F., Bin, Z., Su, H. W. & Zheng, M. L. (2003). *Chin. J. Appl. Chem.* **20**, 365–367.