

2-Chloro-*N'*-(2-chlorobenzylidene)-benzohydrazideDong-Hui Zou,<sup>a\*</sup> Hong Guan<sup>b</sup> and Xiao-Hua Zhang<sup>c</sup><sup>a</sup>College of Life Science and Engineering, Qiqihar University, Qiqihar 161006, People's Republic of China, <sup>b</sup>Qiqihar Medical University, Qiqihar 161006, People's Republic of China, and <sup>c</sup>Liaoning Cheng Da Biotechnology Co Ltd, Shenyang 100044, People's Republic of China

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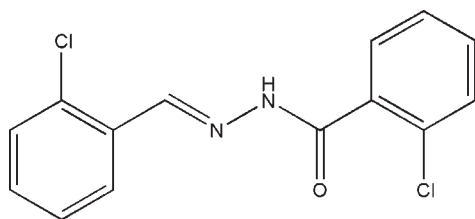
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.038;  $wR$  factor = 0.098; data-to-parameter ratio = 16.4.

The molecule of the title compound,  $\text{C}_{14}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}$ , adopts an *E* configuration about the  $\text{C}=\text{N}$  bond. The dihedral angle between the two benzene rings is  $79.7(2)^\circ$ . In the crystal structure, molecules are linked by intermolecular  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{C}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, forming chains running along the *b* axis.

## Related literature

For the biological activity of hydrazones, see: Küçükgülzel *et al.* (2003); Charkoudian *et al.* (2007); Avaji *et al.* (2009); Kümmerle *et al.* (2009); Raparti *et al.* (2009); Bayrak *et al.* (2009); Hearn *et al.* (2009). For crystal structures of hydrazone compounds, see: Fun *et al.* (2008); Lo & Ng (2009); Ren (2009); Zhang (2009); Wu (2009); Peng & Hou (2008); Mohd Lair *et al.* (2009); Liang & Zou (2009).



## Experimental

## Crystal data

 $\text{C}_{14}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}$  $M_r = 293.14$ Orthorhombic, *Pbca* $a = 11.9336(5)$  Å $b = 9.7471(4)$  Å $c = 22.5840(9)$  Å $V = 2626.93(19)$  Å<sup>3</sup> $Z = 8$ Mo  $K\alpha$  radiation $\mu = 0.49$  mm<sup>-1</sup> $T = 298$  K $0.23 \times 0.21 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min} = 0.897$ ,  $T_{\max} = 0.909$ 

15167 measured reflections

2863 independent reflections

2035 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.045$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.038$  $wR(F^2) = 0.098$  $S = 1.03$ 

2863 reflections

175 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\max} = 0.21$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.36$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O1}^i$	0.91 (1)	1.920 (12)	2.809 (2)	166 (2)
$\text{C7}-\text{H7}\cdots\text{O1}^i$	0.93	2.53	3.301 (2)	141
$\text{C14}-\text{H14}\cdots\text{Cl2}^i$	0.93	2.75	3.620 (2)	156

Symmetry code: (i)  $-x + \frac{3}{2}, y - \frac{1}{2}, z$ .

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2943).

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**supplementary materials**

*Acta Cryst.* (2009). E65, o2871 [ doi:10.1107/S1600536809043803 ]

## 2-Chloro-*N'*-(2-chlorobenzylidene)benzohydrazide

D.-H. Zou, H. Guan and X.-H. Zhang

### Comment

During the past decades, the human population affected with life-treating infectious diseases caused by multidrug-resistant Gram-positive and Gram-negative pathogen bacteria increased to an alarming level around the world. Recently, a great deal of antibacterial agents were used in therapy. Hydrazones are an important component of the Schiff base family. These compounds have been widely used in the fields of antimicrobial, antibacterial and antitumor (Küçükgül *et al.*, 2003; Charkoudian *et al.*, 2007; Avaji *et al.*, 2009; Kümmerle *et al.*, 2009; Raparti *et al.*, 2009; Bayrak *et al.*, 2009; Hearn *et al.*, 2009). In the last few years, crystal structures of a number of hydrazone compounds have been reported (Fun *et al.*, 2008; Lo & Ng, 2009; Ren, 2009; Zhang, 2009). As a continuation of our work in this area (Liang & Zou, 2009), the author reports herein the crystal structure of the title new hydrazone compound.

In the title molecule (Fig. 1), the dihedral angle between the two benzene rings is 79.7 (2)°. The molecule exists in an *E* configuration about the C=N bond. All bond lengths are within normal values and comparable to those observed in related hydrazone compounds (Wu, 2009; Peng & Hou, 2008; Mohd Lair *et al.*, 2009).

In the crystal structure of the title compound, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1), forming chains running along the *b* axis (Fig. 2).

### Experimental

Equimolar quantities (1.0 mmol each) of 2-chlorobenzaldehyde and 2-chlorobenzohydrazide were mixed and refluxed in methanol. The reaction mixture was cooled to room temperature to give a clear colourless solution. Colourless single crystals of the title compound were formed by slow evaporation of the solution in air.

### Refinement

Atom H2 was located in a difference map and refined isotropically, with the N-H distance restrained to 0.90 (1) Å and  $U_{\text{iso}}$  set at 0.08 Å<sup>2</sup>. Other H atoms were placed in calculated positions (C-H = 0.93 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

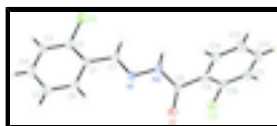


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids for the non-hydrogen atoms. H atoms are shown as spheres of arbitrary radius.

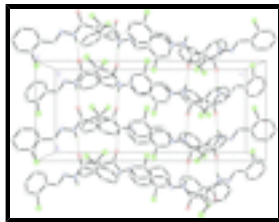


Fig. 2. The packing diagram, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

## 2-Chloro-*N'*-(2-chlorobenzylidene)benzohydrazide

### Crystal data

$C_{14}H_{10}Cl_2N_2O$	$F_{000} = 1200$
$M_r = 293.14$	$D_x = 1.482 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ac 2ab	Cell parameters from 2480 reflections
$a = 11.9336 (5) \text{ \AA}$	$\theta = 2.4\text{--}24.5^\circ$
$b = 9.7471 (4) \text{ \AA}$	$\mu = 0.49 \text{ mm}^{-1}$
$c = 22.5840 (9) \text{ \AA}$	$T = 298 \text{ K}$
$V = 2626.93 (19) \text{ \AA}^3$	Block, colourless
$Z = 8$	$0.23 \times 0.21 \times 0.20 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer	2863 independent reflections
Radiation source: fine-focus sealed tube	2035 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.045$
$T = 298 \text{ K}$	$\theta_{\text{max}} = 27.0^\circ$
$\omega$ scans	$\theta_{\text{min}} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 11$
$T_{\text{min}} = 0.897$ , $T_{\text{max}} = 0.909$	$k = -12 \rightarrow 12$
15167 measured reflections	$l = -28 \rightarrow 28$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.098$	$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.9372P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
2863 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
175 parameters	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$
	Extinction correction: none

Primary atom site location: structure-invariant direct methods

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.79500 (6)	0.47092 (7)	0.48378 (3)	0.0674 (2)
C12	0.53369 (5)	1.04300 (6)	0.72070 (3)	0.05271 (18)
N1	0.84153 (13)	0.81563 (16)	0.59949 (6)	0.0345 (4)
N2	0.78786 (14)	0.79951 (16)	0.65338 (7)	0.0341 (4)
O1	0.78386 (13)	1.02813 (13)	0.67114 (6)	0.0445 (4)
C1	0.90227 (16)	0.7097 (2)	0.51022 (8)	0.0352 (4)
C2	0.88637 (17)	0.6053 (2)	0.46878 (9)	0.0413 (5)
C3	0.9388 (2)	0.6077 (3)	0.41454 (10)	0.0540 (6)
H3	0.9271	0.5370	0.3876	0.065*
C4	1.0084 (2)	0.7148 (3)	0.40032 (10)	0.0560 (6)
H4	1.0434	0.7167	0.3635	0.067*
C5	1.02694 (18)	0.8197 (2)	0.44010 (9)	0.0494 (6)
H5	1.0743	0.8920	0.4303	0.059*
C6	0.97447 (17)	0.8163 (2)	0.49456 (9)	0.0415 (5)
H6	0.9876	0.8867	0.5215	0.050*
C7	0.84564 (16)	0.70741 (19)	0.56775 (8)	0.0359 (4)
H7	0.8126	0.6268	0.5812	0.043*
C8	0.76315 (16)	0.91055 (19)	0.68656 (8)	0.0327 (4)
C9	0.71126 (16)	0.87531 (19)	0.74505 (8)	0.0346 (4)
C10	0.61214 (17)	0.9330 (2)	0.76526 (9)	0.0387 (5)
C11	0.5702 (2)	0.9017 (3)	0.82073 (10)	0.0520 (6)
H11	0.5042	0.9422	0.8339	0.062*
C12	0.6263 (2)	0.8106 (3)	0.85620 (10)	0.0600 (7)
H12	0.5982	0.7897	0.8935	0.072*
C13	0.7236 (2)	0.7499 (3)	0.83710 (10)	0.0570 (6)
H13	0.7606	0.6869	0.8611	0.068*
C14	0.76608 (19)	0.7831 (2)	0.78197 (9)	0.0462 (5)
H14	0.8326	0.7430	0.7694	0.055*
H2	0.768 (2)	0.7142 (14)	0.6655 (11)	0.080*

## supplementary materials

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### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	0.0867 (5)	0.0575 (4)	0.0581 (4)	-0.0282 (3)	0.0204 (3)	-0.0183 (3)
C12	0.0438 (3)	0.0540 (4)	0.0603 (4)	0.0084 (3)	-0.0088 (3)	-0.0094 (3)
N1	0.0413 (9)	0.0334 (9)	0.0288 (8)	0.0033 (7)	0.0049 (7)	0.0008 (7)
N2	0.0447 (10)	0.0279 (8)	0.0297 (8)	0.0004 (7)	0.0066 (7)	-0.0014 (7)
O1	0.0614 (10)	0.0267 (7)	0.0452 (8)	0.0046 (7)	0.0093 (7)	0.0024 (6)
C1	0.0396 (11)	0.0358 (11)	0.0301 (10)	0.0058 (8)	0.0022 (8)	0.0013 (8)
C2	0.0448 (12)	0.0416 (12)	0.0376 (11)	-0.0017 (9)	0.0059 (9)	-0.0040 (9)
C3	0.0608 (15)	0.0597 (15)	0.0415 (12)	-0.0060 (12)	0.0127 (11)	-0.0152 (11)
C4	0.0565 (14)	0.0716 (17)	0.0399 (12)	-0.0003 (12)	0.0174 (11)	-0.0033 (12)
C5	0.0482 (13)	0.0532 (14)	0.0467 (12)	-0.0033 (11)	0.0100 (10)	0.0051 (11)
C6	0.0486 (13)	0.0370 (11)	0.0390 (11)	-0.0009 (9)	0.0038 (9)	0.0007 (9)
C7	0.0452 (11)	0.0308 (10)	0.0318 (10)	0.0007 (9)	0.0034 (8)	0.0015 (8)
C8	0.0354 (10)	0.0285 (10)	0.0341 (10)	0.0027 (8)	-0.0007 (8)	-0.0006 (8)
C9	0.0412 (11)	0.0314 (10)	0.0314 (10)	-0.0012 (8)	0.0024 (8)	-0.0035 (8)
C10	0.0380 (11)	0.0379 (11)	0.0402 (11)	-0.0033 (9)	0.0002 (9)	-0.0109 (9)
C11	0.0460 (13)	0.0633 (15)	0.0467 (13)	-0.0057 (11)	0.0126 (10)	-0.0157 (12)
C12	0.0669 (17)	0.0763 (18)	0.0368 (12)	-0.0104 (14)	0.0154 (12)	0.0003 (12)
C13	0.0686 (16)	0.0625 (15)	0.0398 (12)	0.0039 (13)	0.0043 (11)	0.0107 (11)
C14	0.0535 (13)	0.0460 (13)	0.0391 (11)	0.0066 (10)	0.0070 (10)	0.0025 (10)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C11—C2	1.738 (2)	C5—C6	1.381 (3)
C12—C10	1.743 (2)	C5—H5	0.93
N1—C7	1.276 (2)	C6—H6	0.93
N1—N2	1.384 (2)	C7—H7	0.93
N2—C8	1.349 (2)	C8—C9	1.499 (3)
N2—H2	0.908 (10)	C9—C10	1.387 (3)
O1—C8	1.223 (2)	C9—C14	1.389 (3)
C1—C6	1.395 (3)	C10—C11	1.383 (3)
C1—C2	1.395 (3)	C11—C12	1.371 (3)
C1—C7	1.465 (3)	C11—H11	0.93
C2—C3	1.376 (3)	C12—C13	1.372 (3)
C3—C4	1.373 (3)	C12—H12	0.93
C3—H3	0.93	C13—C14	1.383 (3)
C4—C5	1.379 (3)	C13—H13	0.93
C4—H4	0.93	C14—H14	0.93
C7—N1—N2	114.69 (16)	N1—C7—H7	119.9
C8—N2—N1	119.89 (15)	C1—C7—H7	119.9
C8—N2—H2	120.6 (17)	O1—C8—N2	123.33 (17)
N1—N2—H2	119.5 (17)	O1—C8—C9	123.31 (17)
C6—C1—C2	117.19 (17)	N2—C8—C9	113.33 (16)
C6—C1—C7	121.43 (18)	C10—C9—C14	117.81 (18)
C2—C1—C7	121.39 (18)	C10—C9—C8	123.31 (17)

C3—C2—C1	121.5 (2)	C14—C9—C8	118.85 (17)
C3—C2—C11	118.13 (17)	C11—C10—C9	121.1 (2)
C1—C2—C11	120.29 (15)	C11—C10—C12	117.69 (17)
C4—C3—C2	119.8 (2)	C9—C10—C12	121.17 (15)
C4—C3—H3	120.1	C12—C11—C10	119.7 (2)
C2—C3—H3	120.1	C12—C11—H11	120.1
C3—C4—C5	120.6 (2)	C10—C11—H11	120.1
C3—C4—H4	119.7	C11—C12—C13	120.6 (2)
C5—C4—H4	119.7	C11—C12—H12	119.7
C4—C5—C6	119.3 (2)	C13—C12—H12	119.7
C4—C5—H5	120.3	C12—C13—C14	119.5 (2)
C6—C5—H5	120.3	C12—C13—H13	120.3
C5—C6—C1	121.6 (2)	C14—C13—H13	120.3
C5—C6—H6	119.2	C13—C14—C9	121.3 (2)
C1—C6—H6	119.2	C13—C14—H14	119.4
N1—C7—C1	120.20 (17)	C9—C14—H14	119.4

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2 $\cdots$ O1 <sup>i</sup>	0.91 (1)	1.920 (12)	2.809 (2)	166 (2)
C7—H7 $\cdots$ O1 <sup>i</sup>	0.93	2.53	3.301 (2)	141
C14—H14 $\cdots$ C12 <sup>i</sup>	0.93	2.75	3.620 (2)	156

Symmetry codes: (i)  $-x+3/2, y-1/2, z$ .

Fig. 1

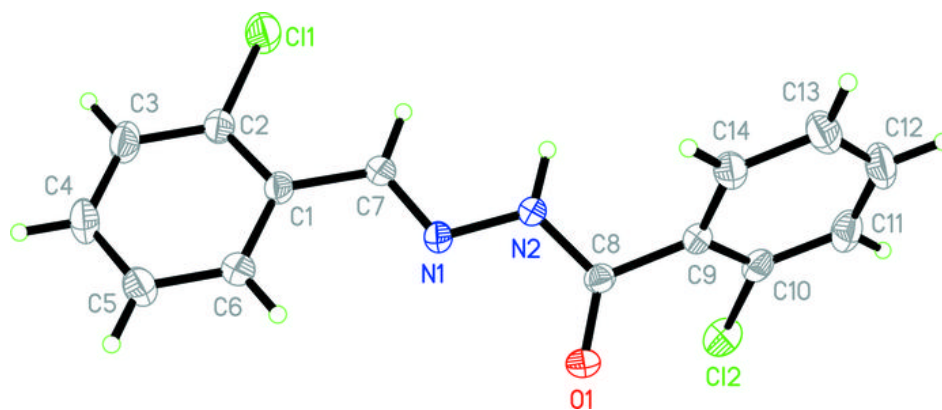




Fig. 2

