Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Chloro-*N*′-(2-hydroxybenzylidene)-benzohydrazide monohydrate

Jiu-Fu Lu,* Suo-Tian Min, Xiao-Hui Ji and Zhong-Hai Dang

School of Chemistry and Environmental Science, Shaanxi University of Technology, Hanzhong 723000, People's Republic of China
Correspondence e-mail: jiufulu@163.com

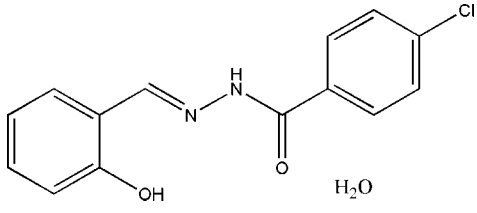
Received 28 July 2008; accepted 31 July 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.069; wR factor = 0.215; data-to-parameter ratio = 15.4.

The asymmetric unit of the title compound, $C_{14}H_{11}ClN_2O_2\cdot H_2O$, contains a Schiff base molecule and a water molecule of crystallization. The dihedral angle between the two aromatic rings is 27.3 (4)°. In the crystal structure, molecules are linked into a two-dimensional network parallel to the *bc* plane by intermolecular O—H···O and N—H···O hydrogen bonds involving the water molecules.

Related literature

For general background on Schiff bases derived from condensation of aldehydes with benzohydrazides, see: Fun *et al.* (2008); Alhadi *et al.* (2008); Ali *et al.* (2007); Zou *et al.* (2004); Shan *et al.* (2008); Bedia *et al.* (2006); Terzioglu & Gürsoy (2003). For related structures, see: Nie (2008); He (2008); Shi *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{11}ClN_2O_2\cdot H_2O$
M_r = 292.71
Monoclinic, $P2_1/c$
a = 22.397 (3) Å
b = 4.853 (2) Å
c = 12.642 (3) Å
β = 97.15 (3)°
V = 1363.4 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 (2) K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.937, T_{max} = 0.945
10537 measured reflections
2946 independent reflections
1251 reflections with $I > 2\sigma(I)$
R_{int} = 0.106

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.214
S = 0.99
2946 reflections
191 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2	0.84 (3)	1.97 (3)	2.800 (4)	170 (5)
O3—H3B···O2^{i}	0.85 (3)	2.07 (3)	2.828 (4)	149 (5)
N2—H2···O3^{ii}	0.90 (1)	1.96 (1)	2.856 (4)	172 (5)
O1—H1···N1	0.82	1.96	2.667 (5)	143

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

The authors acknowledge Shaanxi University of Technology for the research fund.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2647).

References

Alhadi, A. A., Ali, H. M., Puvaneswary, S., Robinson, W. T. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o1584.
Ali, H. M., Zuraini, K., Wan Jefrey, B. & Ng, S. W. (2007). *Acta Cryst.* E**63**, o1729–o1730.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Bedia, K.-K., Elcin, O., Seda, U., Fatma, K., Nathaly, S., Sevim, R. & Dimoglo, A. (2006). *Eur. J. Med. Chem.* **41**, 1253–1261.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fun, H.-K., Patil, P. S., Jebas, S. R., Sujith, K. V. & Kalluraya, B. (2008). *Acta Cryst.* E**64**, o1594–o1595.
He, L. (2008). *Acta Cryst.* E**64**, o82.
Nie, Y. (2008). *Acta Cryst.* E**64**, o471.
Shan, S., Tian, Y.-L., Wang, S.-H., Wang, W.-L. & Xu, Y.-L. (2008). *Acta Cryst.* E**64**, o1363.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shi, X.-F., Liu, C.-Y., Liu, B. & Yuan, C.-C. (2007). *Acta Cryst.* E**63**, o1295–o1296.
Terzioglu, N. & Gürsoy, A. (2003). *Eur. J. Med. Chem.* **38**, 781–786.
Zou, W., Yu, H. & Meng, J. (2004). *Acta Cryst.* E**60**, o671–o673.

supporting information

Acta Cryst. (2008). E**64**, o1694 [doi:10.1107/S1600536808024471]

4-Chloro-*N*′-(2-hydroxybenzylidene)benzohydrazide monohydrate

Jiu-Fu Lu, Suo-Tian Min, Xiao-Hui Ji and Zhong-Hai Dang

S1. Comment

Schiff bases derived from the condensation of aldehydes with benzohydrazides have been widely investigated, either for their structures (Fun *et al.*, 2008; Alhadi *et al.*, 2008; Ali *et al.*, 2007; Zou *et al.*, 2004; Shan *et al.*, 2008) or for their biological properties (Bedia *et al.*, 2006; Terzioglu & Gürsoy, 2003). This study extends the structural study on such compounds.

The asymmetric unit of the title compound consists of a Schiff base molecule and a water molecule of crystallization (Fig. 1). The bond lengths are within normal values (Allen *et al.*, 1987), and comparable to the values observed in related compounds (Nie, 2008; He, 2008; Shi *et al.*, 2007). The dihedral angle between the two aromatic rings in the Schiff base molecule is 27.3 (4)°. An intramolecular O—H···N hydrogen bond is observed.

In the crystal structure, the molecules are linked into a two-dimensional network parallel to the *bc* plane by intermolecular O–H···O and N–H···O hydrogen bonds (Table 1) involving the water molecules (Fig. 2).

S2. Experimental

The title compound was prepared by the Schiff base condensation of salicylaldehyde (0.1 mol) and 4-chloro-benzohydrazide (0.1 mmol) in ethanol (50 ml). The excess ethanol was removed by distillation. The colourless solid formed was filtered and washed with ethanol. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at room temperature.

S3. Refinement

The imino and water H atoms were located in a difference map and refined with N–H, O–H and H···H distances restrained to 0.90 (1), 0.85 (1), and 1.37 (2)Å, respectively. The other H atoms were positioned geometrically [C–H = 0.93 Å and O–H = 0.82Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O1).

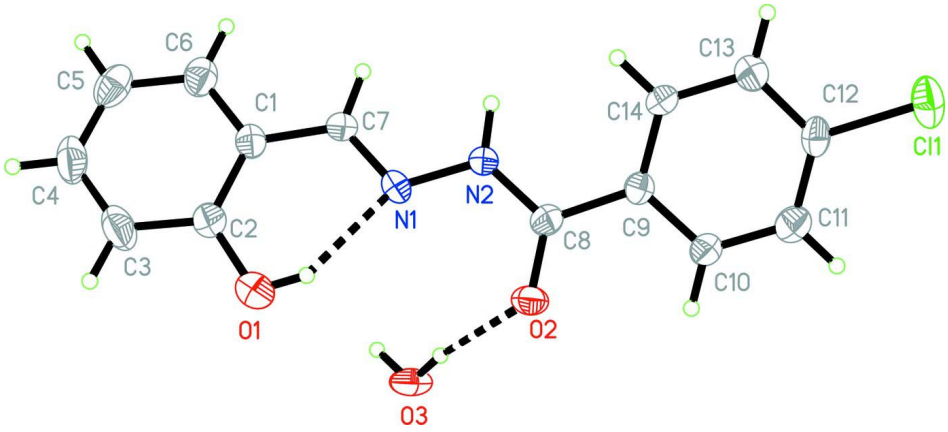


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines indicate hydrogen bonds.

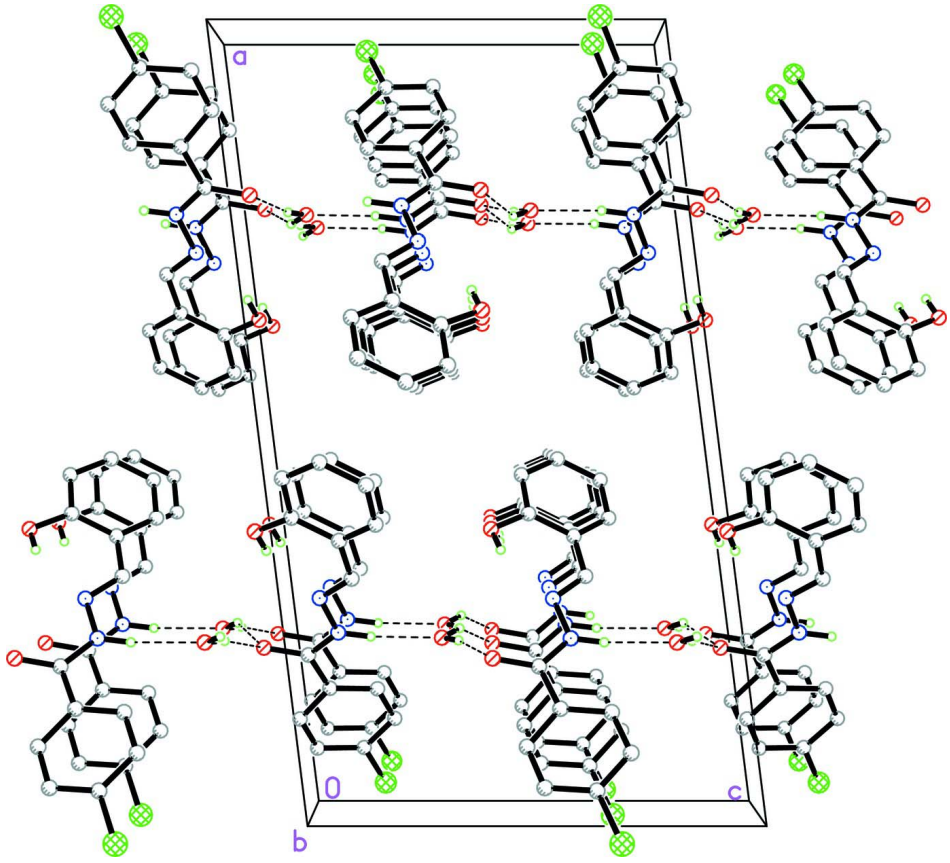


Figure 2

The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

4-Chloro-N′-(2-hydroxybenzylidene)benzohydrazide monohydrate

Crystal data

$C_{14}H_{11}ClN_2O_2·H_2O$
$M_r = 292.71$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 22.397$ (3) Å
$b = 4.853$ (2) Å
$c = 12.642$ (3) Å
$\beta = 97.15$ (3)°
$V = 1363.4$ (7) Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.426$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 600 reflections
$\theta = 2.6$–24.5°
$\mu = 0.29$ mm^{-1}
$T = 298$ K
Block, colourless
0.23 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.937$, $T_{max} = 0.945$
10537 measured reflections
2946 independent reflections
1251 reflections with $I > 2\sigma(I)$
$R_{int} = 0.106$
$\theta_{max} = 27.0°$, $\theta_{min} = 0.9°$
$h = -28 \rightarrow 28$
$k = -6 \rightarrow 6$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.214$
$S = 0.99$
2946 reflections
191 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0902P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.02717 (6)	1.4002 (3)	0.66329 (12)	0.0731 (5)
N2	0.24096 (15)	0.4463 (8)	0.6210 (3)	0.0392 (9)
C8	0.21035 (19)	0.5999 (9)	0.5457 (3)	0.0412 (11)

N1	0.28603 (15)	0.2706 (7)	0.5952 (3)	0.0420 (10)
O2	0.21956 (14)	0.5852 (6)	0.4508 (2)	0.0538 (9)
C9	0.16460 (18)	0.7918 (8)	0.5783 (3)	0.0365 (10)
C14	0.16219 (18)	0.8667 (9)	0.6822 (3)	0.0426 (12)
H14	0.1893	0.7895	0.7359	0.051*
C1	0.35917 (19)	−0.0643 (9)	0.6600 (3)	0.0415 (11)
C7	0.31165 (18)	0.1242 (9)	0.6720 (3)	0.0428 (12)
H7	0.2987	0.1416	0.7388	0.051*
O1	0.36902 (17)	0.0745 (9)	0.4810 (3)	0.0779 (12)
H1	0.3447	0.1897	0.4963	0.117*
C11	0.0808 (2)	1.0889 (10)	0.5252 (4)	0.0537 (13)
H11	0.0531	1.1631	0.4720	0.064*
C12	0.07965 (19)	1.1639 (9)	0.6292 (4)	0.0457 (12)
C13	0.1200 (2)	1.0561 (10)	0.7088 (4)	0.0512 (13)
H13	0.1191	1.1086	0.7793	0.061*
C2	0.3871 (2)	−0.0802 (11)	0.5669 (4)	0.0536 (13)
C10	0.12292 (19)	0.9047 (10)	0.4998 (3)	0.0466 (12)
H10	0.1236	0.8543	0.4290	0.056*
C6	0.3802 (2)	−0.2325 (10)	0.7435 (4)	0.0577 (14)
H6	0.3624	−0.2236	0.8060	0.069*
C4	0.4539 (2)	−0.4315 (13)	0.6486 (5)	0.0726 (17)
H4	0.4851	−0.5558	0.6443	0.087*
C5	0.4271 (2)	−0.4144 (11)	0.7380 (5)	0.0656 (15)
H5	0.4402	−0.5255	0.7962	0.079*
C3	0.4344 (2)	−0.2616 (12)	0.5632 (5)	0.0739 (17)
H3	0.4536	−0.2697	0.5021	0.089*
O3	0.23525 (17)	0.0885 (7)	0.3450 (2)	0.0568 (9)
H2	0.236 (2)	0.445 (11)	0.6905 (12)	0.080*
H3B	0.245 (2)	−0.049 (5)	0.385 (3)	0.080*
H3A	0.235 (2)	0.234 (5)	0.381 (3)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0598 (8)	0.0587 (9)	0.1059 (12)	0.0176 (7)	0.0301 (8)	0.0051 (9)
N2	0.042 (2)	0.044 (2)	0.0329 (19)	0.0072 (18)	0.0065 (17)	0.002 (2)
C8	0.044 (3)	0.040 (3)	0.039 (3)	0.000 (2)	0.003 (2)	0.004 (2)
N1	0.041 (2)	0.042 (2)	0.044 (2)	0.0057 (19)	0.0121 (18)	−0.006 (2)
O2	0.078 (2)	0.050 (2)	0.0345 (18)	0.0109 (18)	0.0142 (16)	0.0034 (16)
C9	0.038 (2)	0.030 (3)	0.041 (3)	−0.002 (2)	0.005 (2)	0.003 (2)
C14	0.045 (3)	0.046 (3)	0.035 (3)	0.005 (2)	−0.001 (2)	0.004 (2)
C1	0.037 (2)	0.038 (3)	0.049 (3)	−0.001 (2)	0.003 (2)	−0.007 (2)
C7	0.044 (3)	0.052 (3)	0.033 (2)	0.005 (2)	0.005 (2)	−0.001 (2)
O1	0.084 (3)	0.098 (3)	0.054 (2)	0.030 (2)	0.0195 (19)	0.002 (2)
C11	0.050 (3)	0.058 (3)	0.053 (3)	0.001 (3)	0.001 (2)	0.005 (3)
C12	0.040 (2)	0.033 (3)	0.065 (3)	0.004 (2)	0.010 (2)	0.007 (2)
C13	0.053 (3)	0.051 (3)	0.050 (3)	0.006 (3)	0.010 (2)	−0.001 (3)
C2	0.051 (3)	0.061 (4)	0.048 (3)	0.009 (3)	0.004 (2)	−0.005 (3)

C10	0.044 (3)	0.054 (3)	0.041 (3)	0.007 (3)	0.003 (2)	0.004 (3)
C6	0.050 (3)	0.055 (3)	0.066 (3)	0.003 (3)	−0.002 (3)	−0.005 (3)
C4	0.051 (3)	0.068 (4)	0.096 (5)	0.019 (3)	−0.001 (3)	−0.024 (4)
C5	0.063 (4)	0.050 (4)	0.077 (4)	−0.001 (3)	−0.019 (3)	−0.002 (3)
C3	0.064 (4)	0.078 (4)	0.083 (4)	0.017 (3)	0.020 (3)	−0.025 (4)
O3	0.091 (2)	0.047 (2)	0.0328 (17)	−0.007 (2)	0.0107 (17)	−0.0014 (17)

Geometric parameters (Å, º)

Cl1—C12	1.735 (4)	C11—C10	1.366 (6)
N2—C8	1.330 (5)	C11—C12	1.367 (6)
N2—N1	1.391 (5)	C11—H11	0.93
N2—H2	0.899 (10)	C12—C13	1.370 (6)
C8—O2	1.245 (5)	C13—H13	0.93
C8—C9	1.481 (6)	C2—C3	1.384 (7)
N1—C7	1.280 (5)	C10—H10	0.93
C9—C14	1.370 (6)	C6—C5	1.380 (7)
C9—C10	1.388 (6)	C6—H6	0.93
C14—C13	1.390 (6)	C4—C5	1.346 (7)
C14—H14	0.93	C4—C3	1.386 (7)
C1—C6	1.371 (6)	C4—H4	0.93
C1—C2	1.401 (6)	C5—H5	0.93
C1—C7	1.426 (6)	C3—H3	0.93
C7—H7	0.93	O3—H3B	0.85 (3)
O1—C2	1.340 (5)	O3—H3A	0.84 (3)
O1—H1	0.82		
C8—N2—N1	120.0 (3)	C11—C12—Cl1	120.7 (4)
C8—N2—H2	126 (3)	C13—C12—Cl1	118.3 (4)
N1—N2—H2	114 (3)	C12—C13—C14	118.8 (4)
O2—C8—N2	121.7 (4)	C12—C13—H13	120.6
O2—C8—C9	120.5 (4)	C14—C13—H13	120.6
N2—C8—C9	117.8 (4)	O1—C2—C3	119.0 (5)
C7—N1—N2	115.6 (3)	O1—C2—C1	121.9 (4)
C14—C9—C10	118.5 (4)	C3—C2—C1	119.1 (5)
C14—C9—C8	123.0 (4)	C11—C10—C9	120.8 (4)
C10—C9—C8	118.4 (4)	C11—C10—H10	119.6
C9—C14—C13	121.1 (4)	C9—C10—H10	119.6
C9—C14—H14	119.5	C1—C6—C5	122.2 (5)
C13—C14—H14	119.5	C1—C6—H6	118.9
C6—C1—C2	117.9 (4)	C5—C6—H6	118.9
C6—C1—C7	119.3 (4)	C5—C4—C3	119.1 (5)
C2—C1—C7	122.8 (4)	C5—C4—H4	120.4
N1—C7—C1	123.0 (4)	C3—C4—H4	120.4
N1—C7—H7	118.5	C4—C5—C6	120.3 (5)
C1—C7—H7	118.5	C4—C5—H5	119.9
C2—O1—H1	109.5	C6—C5—H5	119.9
C10—C11—C12	119.8 (4)	C2—C3—C4	121.4 (5)

C10—C11—H11	120.1	C2—C3—H3	119.3
C12—C11—H11	120.1	C4—C3—H3	119.3
C11—C12—C13	121.0 (4)	H3B—O3—H3A	111 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2	0.84 (3)	1.97 (3)	2.800 (4)	170 (5)
O3—H3*B*···O2^{i}	0.85 (3)	2.07 (3)	2.828 (4)	149 (5)
N2—H2···O3^{ii}	0.90 (1)	1.96 (1)	2.856 (4)	172 (5)
O1—H1···N1	0.82	1.96	2.667 (5)	143

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