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N′-(2-Hydroxybenzylidene)-2-methoxybenzohydrazide monohydrate

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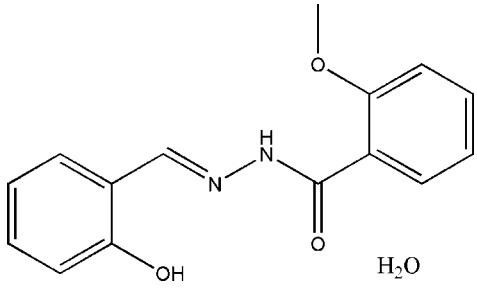
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.130; data-to-parameter ratio = 9.0.

In the title compound, $C_{15}H_{14}N_2O_3\cdot H_2O$, the Schiff base molecule is approximately planar, with a dihedral angle between the two aromatic rings of 10.2 (3)°. The molecular structure is stabilized by O—H···N and N—H···O hydrogen bonds. In the crystal structure, the Schiff base and water molecules are linked together by intermolecular O—H···O hydrogen bonds, forming chains parallel to the *a* axis.

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

$C_{15}H_{14}N_2O_3\cdot H_2O$
M_r = 288.30
Orthorhombic, $P2_12_12_1$
a = 4.761 (2) Å
b = 14.035 (3) Å
c = 21.073 (4) Å
V = 1408.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.17 × 0.16 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.983, T_{max} = 0.985
11662 measured reflections
1808 independent reflections
1345 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.130
S = 1.06
1808 reflections
201 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.97	2.669 (3)	143
N2—H2···O3	0.90 (1)	1.97 (3)	2.629 (3)	129 (3)
O4—H4*B*···O2	0.88 (3)	2.01 (3)	2.880 (4)	171 (3)
O4—H4*A*···O2^{i}	0.88 (3)	2.04 (2)	2.893 (4)	165 (4)

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2646).

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supporting information

Acta Cryst. (2008). E**64**, o1693 [doi:10.1107/S1600536808024483]

N′-(2-Hydroxybenzylidene)-2-methoxybenzohydrazide 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. We report here the crystal structure of the title new Schiff base compound.

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 are comparable to the values observed in similar compounds (Nie, 2008; He, 2008; Shi *et al.*, 2007). The dihedral angle between the two aromatic rings in the Schiff base molecule is 10.2 (3)°, indicating that the molecule is approximately coplanar. The molecular structure is stabilized by O—H···N and N—H···O hydrogen bonds.

In the crystal structure (Fig. 2), the Schiff base and water molecules are linked into chains running parallel to the *a* axis by intermolecular O—H···O hydrogen bonds (Table 1).

S2. Experimental

The title compound was prepared by the Schiff base condensation of salicylaldehyde (0.1 mol) and 2-methoxybenzohydrazide (0.1 mmol) in ethanol (50 ml). The excess ethanol was removed by distillation. The colourless solid obtained was filtered and washed with ethanol. Single crystals suitable for X-ray diffraction were grown by slow evaporation from 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 = 0.93-0.96 Å and O–H = 0.82 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C15 and O1). In the absence of significant anomalous scattering, Friedel pairs were merged.

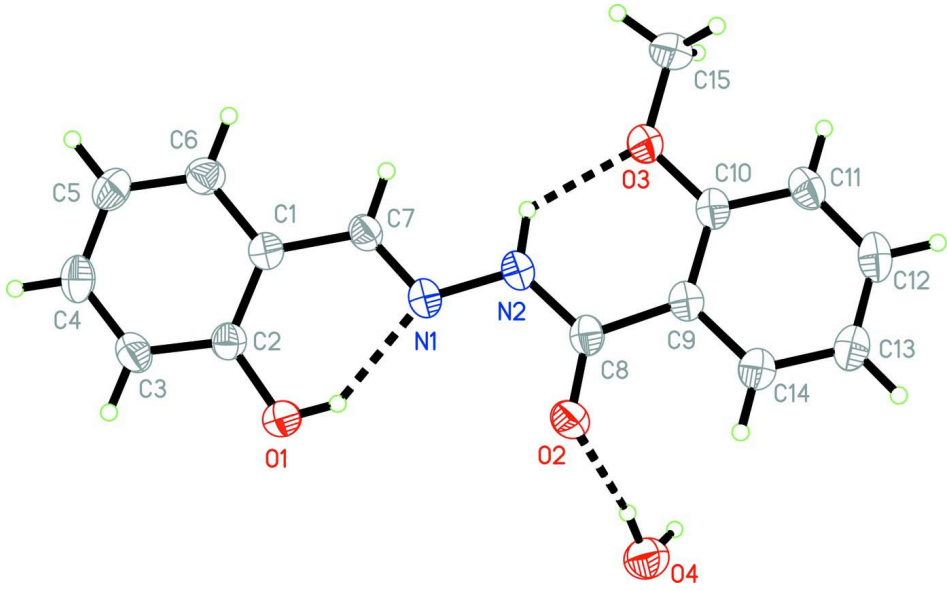

Figure 1

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

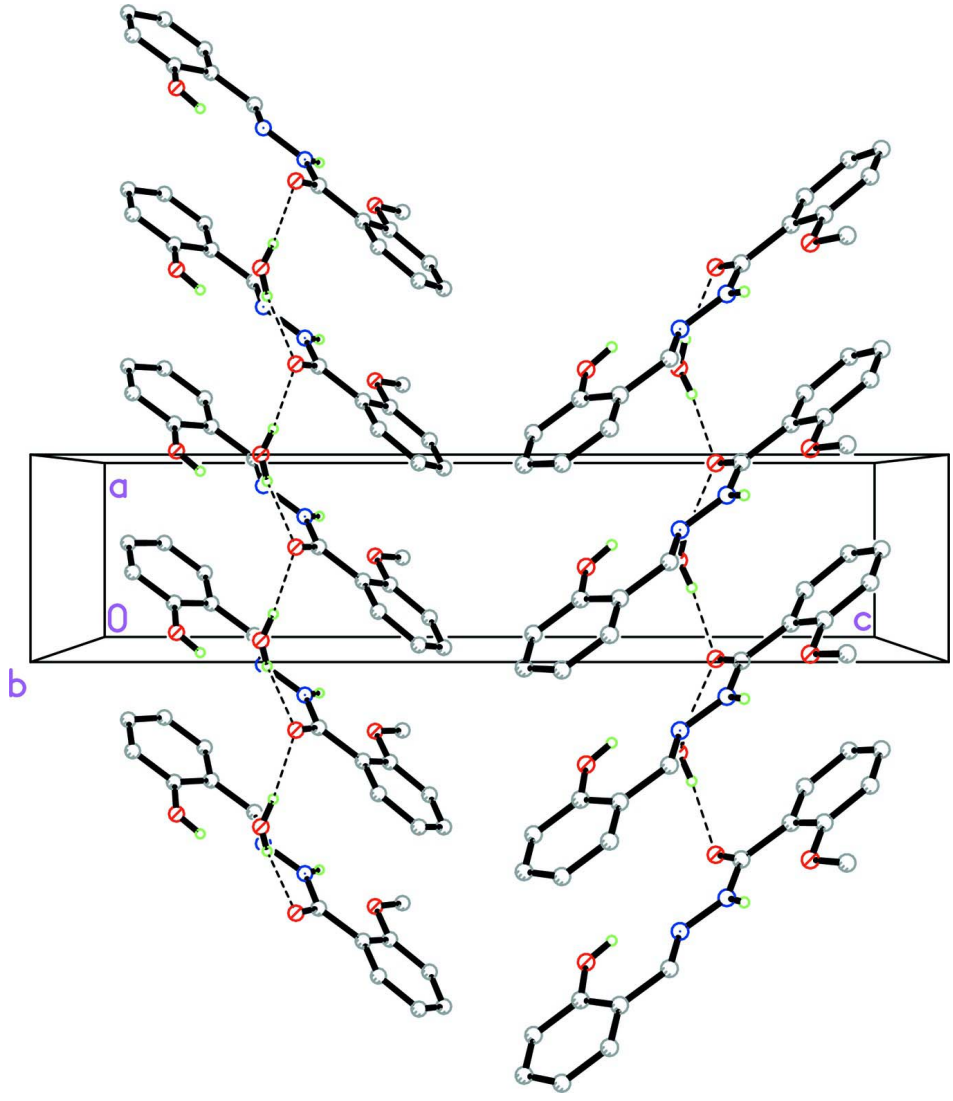

Figure 2

The crystal packing of the title compound, viewed approximately along the *b* axis.

N′-(2-Hydroxybenzylidene)-2-methoxybenzohydrazide monohydrate

Crystal data

$C_{15}H_{14}N_2O_3 \cdot H_2O$
$M_r = 288.30$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.761\ (2)$ Å
$b = 14.035\ (3)$ Å
$c = 21.073\ (4)$ Å
$V = 1408.1\ (7)$ Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.360$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1886 reflections
$\theta = 2.5$–$24.3°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.17 × 0.16 × 0.15 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} = 0.983, T_{max} = 0.985
11662 measured reflections
1808 independent reflections
1345 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.0°, θ_{min} = 1.7°
h = −6→6
k = −17→17
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.130
S = 1.06
1808 reflections
201 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
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.0505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.0565 (6)	0.25999 (15)	0.11044 (10)	0.0662 (7)
H1	0.9443	0.2516	0.1394	0.099*
O2	0.5284 (6)	0.30810 (15)	0.26095 (10)	0.0632 (7)
O3	0.4681 (5)	0.04698 (14)	0.35246 (10)	0.0600 (6)
O4	0.0300 (7)	0.40911 (16)	0.22254 (13)	0.0761 (8)
N1	0.8661 (5)	0.17231 (17)	0.21429 (11)	0.0447 (6)
N2	0.6938 (6)	0.15858 (18)	0.26624 (11)	0.0475 (6)
C1	1.2024 (6)	0.1040 (2)	0.14441 (13)	0.0430 (7)
C2	1.2117 (7)	0.1808 (2)	0.10233 (13)	0.0454 (7)
C3	1.3847 (8)	0.1756 (2)	0.04953 (14)	0.0596 (10)
H3	1.3908	0.2266	0.0214	0.072*
C4	1.5436 (8)	0.0984 (2)	0.03827 (15)	0.0614 (9)
H4	1.6573	0.0968	0.0024	0.074*
C5	1.5411 (8)	0.0215 (2)	0.07896 (15)	0.0617 (9)
H5	1.6533	−0.0314	0.0711	0.074*

C6	1.3700 (8)	0.0247 (2)	0.13124 (15)	0.0539 (8)
H6	1.3654	−0.0272	0.1586	0.065*
C7	1.0217 (7)	0.10236 (19)	0.19971 (13)	0.0450 (7)
H7	1.0197	0.0484	0.2253	0.054*
C8	0.5265 (7)	0.2299 (2)	0.28622 (13)	0.0457 (7)
C9	0.3359 (7)	0.2092 (2)	0.34123 (13)	0.0429 (7)
C10	0.3100 (7)	0.1214 (2)	0.37297 (13)	0.0470 (7)
C11	0.1233 (7)	0.1132 (3)	0.42336 (14)	0.0573 (9)
H11	0.1055	0.0553	0.4445	0.069*
C12	−0.0358 (8)	0.1904 (3)	0.44229 (15)	0.0637 (9)
H12	−0.1616	0.1838	0.4758	0.076*
C13	−0.0103 (8)	0.2763 (2)	0.41233 (14)	0.0565 (8)
H13	−0.1165	0.3283	0.4255	0.068*
C14	0.1751 (7)	0.2848 (2)	0.36233 (14)	0.0509 (8)
H14	0.1925	0.3435	0.3422	0.061*
C15	0.4542 (10)	−0.0415 (2)	0.38602 (17)	0.0750 (12)
H15A	0.4918	−0.0306	0.4302	0.112*
H15B	0.5913	−0.0847	0.3691	0.112*
H15C	0.2700	−0.0684	0.3813	0.112*
H2	0.695 (9)	0.0996 (11)	0.2825 (15)	0.080*
H4A	−0.113 (5)	0.371 (2)	0.2284 (19)	0.080*
H4B	0.169 (5)	0.373 (2)	0.2359 (18)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0823 (19)	0.0551 (13)	0.0613 (14)	0.0192 (14)	0.0190 (13)	0.0106 (10)
O2	0.0598 (15)	0.0610 (13)	0.0688 (14)	0.0056 (14)	0.0168 (14)	0.0188 (11)
O3	0.0623 (15)	0.0557 (12)	0.0621 (13)	0.0040 (12)	0.0182 (13)	0.0086 (10)
O4	0.0771 (18)	0.0626 (15)	0.0885 (18)	0.0020 (16)	0.0056 (18)	0.0012 (13)
N1	0.0417 (14)	0.0533 (15)	0.0390 (13)	−0.0045 (13)	0.0031 (12)	−0.0012 (11)
N2	0.0474 (15)	0.0540 (15)	0.0412 (13)	−0.0037 (14)	0.0074 (13)	0.0013 (11)
C1	0.0423 (17)	0.0448 (15)	0.0418 (15)	−0.0052 (14)	−0.0015 (14)	−0.0042 (13)
C2	0.0482 (18)	0.0461 (16)	0.0417 (15)	−0.0004 (16)	0.0002 (14)	−0.0049 (13)
C3	0.069 (2)	0.059 (2)	0.0506 (19)	−0.002 (2)	0.0155 (17)	0.0066 (15)
C4	0.060 (2)	0.075 (2)	0.0495 (18)	0.000 (2)	0.0131 (17)	−0.0117 (17)
C5	0.063 (2)	0.0592 (19)	0.063 (2)	0.0121 (19)	0.0074 (19)	−0.0126 (17)
C6	0.065 (2)	0.0448 (16)	0.0517 (17)	0.0021 (17)	0.0014 (17)	−0.0021 (14)
C7	0.0477 (18)	0.0438 (15)	0.0434 (15)	−0.0057 (16)	0.0056 (15)	0.0007 (12)
C8	0.0374 (17)	0.0563 (17)	0.0433 (15)	−0.0044 (17)	0.0000 (15)	−0.0030 (14)
C9	0.0359 (16)	0.0546 (17)	0.0381 (14)	−0.0061 (14)	−0.0052 (14)	−0.0049 (13)
C10	0.0400 (17)	0.0591 (18)	0.0420 (15)	−0.0043 (16)	0.0003 (14)	−0.0050 (14)
C11	0.053 (2)	0.070 (2)	0.0495 (18)	−0.0070 (19)	0.0073 (16)	0.0069 (16)
C12	0.054 (2)	0.087 (2)	0.0494 (18)	−0.005 (2)	0.0116 (18)	−0.0080 (17)
C13	0.048 (2)	0.071 (2)	0.0506 (17)	0.0055 (19)	0.0003 (18)	−0.0131 (16)
C14	0.0474 (18)	0.0572 (18)	0.0482 (17)	−0.0020 (17)	−0.0032 (17)	−0.0058 (15)
C15	0.085 (3)	0.064 (2)	0.075 (2)	0.012 (2)	0.012 (2)	0.0219 (18)

Geometric parameters (Å, º)

O1—C2	1.346 (4)	C5—C6	1.371 (4)
O1—H1	0.8200	C5—H5	0.93
O2—C8	1.220 (3)	C6—H6	0.93
O3—C10	1.358 (4)	C7—H7	0.93
O3—C15	1.430 (4)	C8—C9	1.501 (4)
O4—H4A	0.88 (3)	C9—C14	1.383 (4)
O4—H4B	0.88 (3)	C9—C10	1.407 (4)
N1—C7	1.268 (3)	C10—C11	1.389 (4)
N1—N2	1.381 (3)	C11—C12	1.380 (5)
N2—C8	1.347 (4)	C11—H11	0.93
N2—H2	0.897 (10)	C12—C13	1.366 (5)
C1—C6	1.397 (4)	C12—H12	0.93
C1—C2	1.397 (4)	C13—C14	1.380 (4)
C1—C7	1.449 (4)	C13—H13	0.93
C2—C3	1.386 (4)	C14—H14	0.93
C3—C4	1.343 (5)	C15—H15A	0.96
C3—H3	0.93	C15—H15B	0.96
C4—C5	1.378 (4)	C15—H15C	0.96
C4—H4	0.93		

C2—O1—H1	109.5	O2—C8—N2	121.9 (3)
C10—O3—C15	119.0 (3)	O2—C8—C9	121.1 (3)
H4A—O4—H4B	101.2 (19)	N2—C8—C9	117.0 (3)
C7—N1—N2	115.5 (2)	C14—C9—C10	118.1 (3)
C8—N2—N1	119.7 (2)	C14—C9—C8	115.7 (3)
C8—N2—H2	125 (3)	C10—C9—C8	126.2 (3)
N1—N2—H2	115 (3)	O3—C10—C11	122.3 (3)
C6—C1—C2	118.1 (3)	O3—C10—C9	118.2 (3)
C6—C1—C7	119.1 (3)	C11—C10—C9	119.5 (3)
C2—C1—C7	122.8 (3)	C12—C11—C10	120.5 (3)
O1—C2—C3	118.1 (3)	C12—C11—H11	119.8
O1—C2—C1	122.7 (3)	C10—C11—H11	119.8
C3—C2—C1	119.2 (3)	C13—C12—C11	120.7 (3)
C4—C3—C2	121.3 (3)	C13—C12—H12	119.7
C4—C3—H3	119.4	C11—C12—H12	119.7
C2—C3—H3	119.4	C12—C13—C14	119.1 (3)
C3—C4—C5	121.1 (3)	C12—C13—H13	120.4
C3—C4—H4	119.4	C14—C13—H13	120.4
C5—C4—H4	119.4	C13—C14—C9	122.2 (3)
C6—C5—C4	118.7 (3)	C13—C14—H14	118.9
C6—C5—H5	120.7	C9—C14—H14	118.9
C4—C5—H5	120.7	O3—C15—H15A	109.5
C5—C6—C1	121.7 (3)	O3—C15—H15B	109.5
C5—C6—H6	119.2	H15A—C15—H15B	109.5
C1—C6—H6	119.2	O3—C15—H15C	109.5
N1—C7—C1	122.0 (3)	H15A—C15—H15C	109.5

N1—C7—H7	119.0	H15B—C15—H15C	109.5
C1—C7—H7	119.0		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.97	2.669 (3)	143
N2—H2···O3	0.90 (1)	1.97 (3)	2.629 (3)	129 (3)
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Symmetry code: (i) *x*−1, *y*, *z*.