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***N'*-(2-Chloro-5-nitrobenzylidene)-3-hydroxybenzohydrazide methanol solvate**

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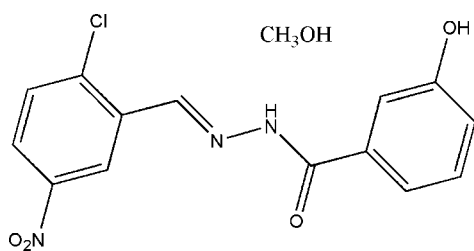
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.045; wR factor = 0.122; data-to-parameter ratio = 14.9.

In the title compound, $\text{C}_{14}\text{H}_{10}\text{ClN}_3\text{O}_4 \cdot \text{CH}_3\text{OH}$, the dihedral angle between the two benzene rings is 33.9 (2)°. In the crystal structure, the methanol solvent molecules are linked to the Schiff base molecules through intermolecular $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds. Molecules are further linked through intermolecular $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds, forming chains running along the b axis.

Related literature

For related structures, see: Zhou & Tang (2007); Zhou & Xiao (2007). For related literature, see: Ali *et al.* (2007); Butcher *et al.* (2007); He (2008); Jing & Yu (2007); Nie (2008).



Experimental

Crystal data

 $\text{C}_{14}\text{H}_{10}\text{ClN}_3\text{O}_4 \cdot \text{CH}_4\text{O}$
 $M_r = 351.74$

 Monoclinic, $P2_1/c$
 $a = 7.716$ (3) Å

 $b = 11.945$ (2) Å
 $c = 17.650$ (3) Å
 $\beta = 99.886$ (2)°
 $V = 1602.6$ (7) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 0.27$ mm⁻¹
 $T = 298$ (2) K
 $0.27 \times 0.23 \times 0.22$ mm

Data collection

 Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.931$, $T_{\max} = 0.943$

 12656 measured reflections
 3316 independent reflections
 2396 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.121$
 $S = 1.01$
 3316 reflections
 223 parameters

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.18$ e Å⁻³
 $\Delta\rho_{\min} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O4}-\text{H4} \cdots \text{O3}^i$	0.82	1.91	2.7237 (19)	169
$\text{O4}-\text{H4} \cdots \text{N2}^i$	0.82	2.62	3.118 (2)	120
$\text{O5}-\text{H5} \cdots \text{O3}^i$	0.82	2.00	2.817 (2)	175
$\text{N3}-\text{H3B} \cdots \text{O5}$	0.81 (3)	2.05 (3)	2.854 (2)	173 (3)

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

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; 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: RZ2226).

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supplementary materials

Acta Cryst. (2008). E64, o1383 [doi:10.1107/S1600536808019636]

N'-(2-Chloro-5-nitrobenzylidene)-3-hydroxybenzohydrazide methanol solvate

Z. Zhou

Comment

Recently, we have reported two metal complexes with Schiff base ligands (Zhou & Tang, 2007; Zhou & Xiao, 2007). We report herein the crystal structure of the title Schiff base compound (Fig. 1).

The title compound consists of a Schiff base molecule and a methanol molecule of crystallization. The dihedral angle between the two benzene rings is 33.9 (2)°. All bond lengths are comparable to those found in similar compounds (Ali *et al.*, 2007; Nie, 2008; He, 2008; Butcher *et al.*, 2007; Jing & Yu, 2007). In the crystal structure, the methanol molecules are linked to the Schiff base molecules through intermolecular N—H···O and O—H···O hydrogen bonds (Table 1). Molecules are further linked through intermolecular O—H···O and O—H···N hydrogen bonds to form chains running along the *b* axis (Fig. 2).

Experimental

2-Chloro-5-nitrobenzaldehyde (1.0 mmol, 167.1 mg) and 3-hydroxybenzohydrazide (1.0 mmol, 152.1 mg) were dissolved in methanol (30 ml). The mixture was stirred at reflux for 30 min to give a colourless solution. After keeping the solution in air for a few days, colourless block-shaped crystals were formed.

Refinement

H3B was located in a difference Fourier map and refined isotropically, with $U_{\text{iso}}(\text{H})$ fixed at 0.08 Å². Other H atoms were positioned geometrically and refined using a riding model with O—H = 0.92 Å, C—H = 0.93–0.96 Å, and with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C}, \text{O})$.

Figures

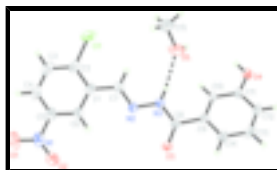


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. Hydrogen bond is shown as a dashed line.

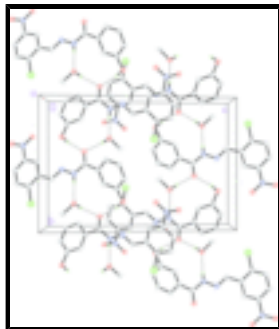


Fig. 2. The crystal packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

***N'*-(2-Chloro-5-nitrobenzylidene)-3-hydroxybenzohydrazide methanol solvate**

Crystal data

$C_{14}H_{10}ClN_3O_4 \cdot CH_4O$

$M_r = 351.74$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.716$ (3) Å

$b = 11.945$ (2) Å

$c = 17.650$ (3) Å

$\beta = 99.886$ (2)°

$V = 1602.6$ (7) Å³

$Z = 4$

$F_{000} = 728$

$D_x = 1.458$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2947 reflections

$\theta = 2.3$ – 24.5 °

$\mu = 0.27$ mm⁻¹

$T = 298$ (2) K

Block, colourless

$0.27 \times 0.23 \times 0.22$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2001)

$T_{\min} = 0.931$, $T_{\max} = 0.943$

12656 measured reflections

3316 independent reflections

2396 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\text{max}} = 26.5$ °

$\theta_{\text{min}} = 2.1$ °

$h = -9 \rightarrow 9$

$k = -14 \rightarrow 14$

$l = -21 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.121$

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

$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.2859P]$

$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3316 reflections	$(\Delta/\sigma)_{\max} < 0.001$
223 parameters	$\Delta\rho_{\max} = 0.18 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.27705 (9)	0.68944 (5)	0.42450 (4)	0.0774 (2)
O1	-0.1188 (3)	1.16001 (18)	0.30340 (10)	0.0978 (7)
O2	0.0033 (3)	1.21390 (16)	0.41618 (12)	0.0859 (6)
O3	0.4707 (2)	1.09327 (11)	0.70885 (8)	0.0623 (4)
O4	0.6995 (2)	0.71117 (11)	0.91382 (8)	0.0607 (4)
H4	0.6479	0.6690	0.8808	0.091*
O5	0.6192 (3)	0.69826 (13)	0.66034 (11)	0.0897 (6)
H5	0.5907	0.6645	0.6968	0.135*
N1	-0.0240 (3)	1.14400 (19)	0.36561 (12)	0.0652 (5)
N2	0.3857 (2)	0.95587 (12)	0.58923 (8)	0.0428 (4)
N3	0.4964 (2)	0.92397 (13)	0.65533 (9)	0.0424 (4)
C1	0.2405 (2)	0.90699 (16)	0.46380 (10)	0.0439 (5)
C2	0.1934 (3)	0.82357 (18)	0.40857 (12)	0.0534 (5)
C3	0.0788 (3)	0.8448 (2)	0.34054 (13)	0.0684 (7)
H3	0.0502	0.7880	0.3045	0.082*
C4	0.0082 (3)	0.9485 (2)	0.32639 (12)	0.0663 (7)
H4A	-0.0690	0.9633	0.2810	0.080*
C5	0.0531 (3)	1.03136 (19)	0.38052 (11)	0.0533 (5)
C6	0.1661 (3)	1.01296 (17)	0.44857 (10)	0.0468 (5)
H6	0.1927	1.0705	0.4841	0.056*
C7	0.3601 (3)	0.88397 (16)	0.53602 (11)	0.0460 (5)
H7	0.4179	0.8154	0.5428	0.055*
C8	0.5280 (2)	0.99647 (15)	0.71415 (10)	0.0429 (4)
C9	0.6354 (2)	0.95567 (15)	0.78653 (10)	0.0409 (4)
C10	0.6158 (2)	0.84831 (15)	0.81342 (10)	0.0414 (4)
H10	0.5366	0.7992	0.7849	0.050*

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C11	0.7141 (3)	0.81385 (16)	0.88285 (11)	0.0451 (5)
C12	0.8325 (3)	0.88781 (18)	0.92424 (11)	0.0536 (5)
H12	0.9003	0.8652	0.9704	0.064*
C13	0.8499 (3)	0.99430 (19)	0.89738 (12)	0.0591 (6)
H13	0.9295	1.0432	0.9259	0.071*
C14	0.7518 (3)	1.03021 (17)	0.82898 (11)	0.0511 (5)
H14	0.7633	1.1029	0.8116	0.061*
C15	0.6536 (4)	0.6218 (2)	0.60542 (17)	0.0899 (9)
H15A	0.6769	0.6613	0.5609	0.135*
H15B	0.5535	0.5739	0.5911	0.135*
H15C	0.7542	0.5775	0.6263	0.135*
H3B	0.538 (3)	0.862 (2)	0.6593 (14)	0.080*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0721 (4)	0.0661 (4)	0.0918 (5)	0.0006 (3)	0.0077 (3)	-0.0362 (3)
O1	0.1037 (15)	0.1191 (16)	0.0612 (11)	0.0065 (12)	-0.0124 (10)	0.0357 (11)
O2	0.0977 (14)	0.0643 (11)	0.0857 (13)	0.0020 (10)	-0.0123 (11)	0.0069 (10)
O3	0.0989 (12)	0.0348 (8)	0.0464 (8)	0.0086 (7)	-0.0068 (8)	-0.0028 (6)
O4	0.0881 (12)	0.0414 (8)	0.0441 (8)	-0.0011 (7)	-0.0130 (7)	0.0061 (6)
O5	0.1570 (19)	0.0489 (10)	0.0750 (12)	0.0195 (10)	0.0527 (12)	0.0041 (8)
N1	0.0607 (12)	0.0783 (14)	0.0543 (12)	-0.0043 (10)	0.0038 (10)	0.0231 (11)
N2	0.0519 (10)	0.0387 (8)	0.0355 (8)	-0.0009 (7)	0.0013 (7)	-0.0009 (7)
N3	0.0523 (10)	0.0363 (8)	0.0357 (8)	0.0010 (7)	-0.0005 (7)	-0.0004 (7)
C1	0.0437 (11)	0.0531 (12)	0.0356 (10)	-0.0079 (8)	0.0087 (8)	-0.0059 (8)
C2	0.0507 (12)	0.0624 (13)	0.0489 (12)	-0.0078 (10)	0.0132 (10)	-0.0157 (10)
C3	0.0644 (15)	0.0928 (19)	0.0463 (13)	-0.0128 (14)	0.0050 (11)	-0.0305 (13)
C4	0.0610 (14)	0.097 (2)	0.0378 (11)	-0.0051 (13)	0.0000 (10)	-0.0035 (12)
C5	0.0506 (12)	0.0699 (14)	0.0396 (11)	-0.0102 (10)	0.0080 (9)	0.0053 (10)
C6	0.0508 (11)	0.0549 (12)	0.0343 (10)	-0.0117 (9)	0.0061 (8)	-0.0001 (8)
C7	0.0541 (12)	0.0415 (10)	0.0413 (10)	-0.0005 (9)	0.0054 (9)	-0.0035 (8)
C8	0.0526 (11)	0.0343 (10)	0.0403 (10)	-0.0041 (8)	0.0041 (9)	-0.0002 (8)
C9	0.0476 (11)	0.0382 (10)	0.0359 (9)	-0.0012 (8)	0.0041 (8)	-0.0030 (7)
C10	0.0477 (11)	0.0377 (10)	0.0359 (10)	-0.0013 (8)	-0.0012 (8)	-0.0065 (8)
C11	0.0540 (12)	0.0415 (11)	0.0376 (10)	0.0039 (8)	0.0020 (9)	-0.0016 (8)
C12	0.0553 (13)	0.0621 (13)	0.0379 (10)	-0.0032 (10)	-0.0075 (9)	-0.0019 (9)
C13	0.0626 (14)	0.0634 (14)	0.0462 (12)	-0.0232 (11)	-0.0049 (10)	-0.0094 (10)
C14	0.0627 (13)	0.0434 (11)	0.0449 (11)	-0.0141 (9)	0.0026 (10)	-0.0020 (9)
C15	0.109 (2)	0.0755 (18)	0.095 (2)	0.0083 (16)	0.0456 (18)	-0.0195 (16)

Geometric parameters (\AA , $^\circ$)

C11—C2	1.732 (2)	C4—C5	1.378 (3)
O1—N1	1.225 (2)	C4—H4A	0.9300
O2—N1	1.214 (3)	C5—C6	1.375 (3)
O3—C8	1.236 (2)	C6—H6	0.9300
O4—C11	1.355 (2)	C7—H7	0.9300
O4—H4	0.8200	C8—C9	1.481 (2)

O5—C15	1.390 (3)	C9—C10	1.385 (3)
O5—H5	0.8200	C9—C14	1.389 (3)
N1—C5	1.477 (3)	C10—C11	1.388 (3)
N2—C7	1.263 (2)	C10—H10	0.9300
N2—N3	1.376 (2)	C11—C12	1.385 (3)
N3—C8	1.342 (2)	C12—C13	1.372 (3)
N3—H3B	0.81 (3)	C12—H12	0.9300
C1—C6	1.397 (3)	C13—C14	1.379 (3)
C1—C2	1.398 (3)	C13—H13	0.9300
C1—C7	1.466 (3)	C14—H14	0.9300
C2—C3	1.387 (3)	C15—H15A	0.9600
C3—C4	1.358 (4)	C15—H15B	0.9600
C3—H3	0.9300	C15—H15C	0.9600
C11—O4—H4	109.5	C1—C7—H7	119.5
C15—O5—H5	109.5	O3—C8—N3	122.02 (17)
O2—N1—O1	123.6 (2)	O3—C8—C9	120.89 (16)
O2—N1—C5	118.83 (18)	N3—C8—C9	117.09 (16)
O1—N1—C5	117.5 (2)	C10—C9—C14	120.50 (17)
C7—N2—N3	115.93 (16)	C10—C9—C8	121.50 (16)
C8—N3—N2	118.75 (15)	C14—C9—C8	117.94 (17)
C8—N3—H3B	120.6 (18)	C9—C10—C11	120.11 (17)
N2—N3—H3B	120.6 (18)	C9—C10—H10	119.9
C6—C1—C2	117.57 (18)	C11—C10—H10	119.9
C6—C1—C7	120.92 (17)	O4—C11—C12	117.23 (17)
C2—C1—C7	121.49 (18)	O4—C11—C10	123.60 (17)
C3—C2—C1	121.6 (2)	C12—C11—C10	119.16 (18)
C3—C2—C11	118.32 (17)	C13—C12—C11	120.26 (18)
C1—C2—C11	120.09 (16)	C13—C12—H12	119.9
C4—C3—C2	120.1 (2)	C11—C12—H12	119.9
C4—C3—H3	119.9	C12—C13—C14	121.29 (18)
C2—C3—H3	119.9	C12—C13—H13	119.4
C3—C4—C5	118.8 (2)	C14—C13—H13	119.4
C3—C4—H4A	120.6	C13—C14—C9	118.66 (19)
C5—C4—H4A	120.6	C13—C14—H14	120.7
C6—C5—C4	122.5 (2)	C9—C14—H14	120.7
C6—C5—N1	118.48 (19)	O5—C15—H15A	109.5
C4—C5—N1	119.0 (2)	O5—C15—H15B	109.5
C5—C6—C1	119.39 (19)	H15A—C15—H15B	109.5
C5—C6—H6	120.3	O5—C15—H15C	109.5
C1—C6—H6	120.3	H15A—C15—H15C	109.5
N2—C7—C1	120.94 (18)	H15B—C15—H15C	109.5
N2—C7—H7	119.5		

Hydrogen-bond geometry (Å, °)

<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>
O4—H4 \cdots O3 ⁱ	0.82	1.91	2.7237 (19)	169
O4—H4 \cdots N2 ⁱ	0.82	2.62	3.118 (2)	120

supplementary materials

O5—H5···O3 ⁱ	0.82	2.00	2.817 (2)	175
N3—H3B···O5	0.81 (3)	2.05 (3)	2.854 (2)	173 (3)

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

Fig. 1

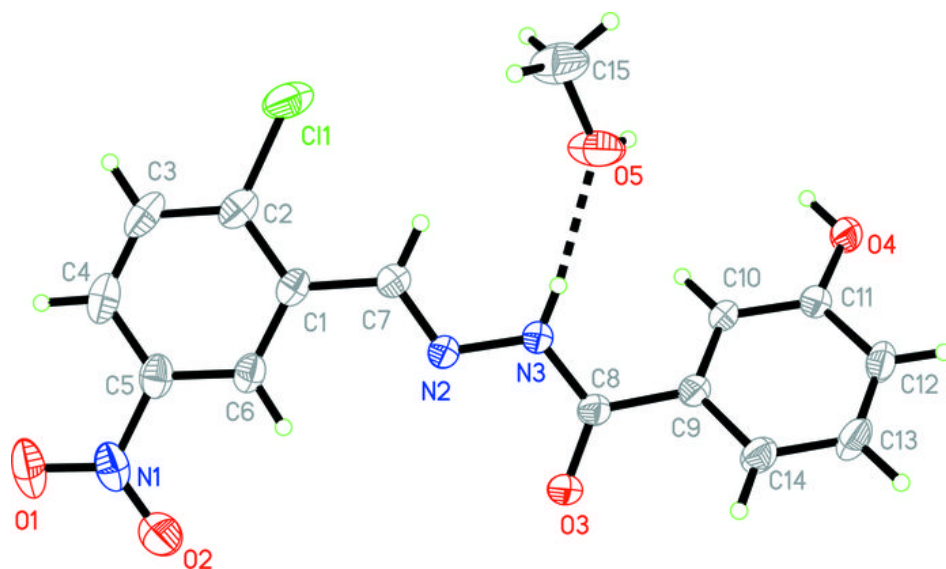


Fig. 2

