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Polymorph of (*E*)-*N*′-(4-chlorobenzylidene)-isonicotinohydrazide monohydrate

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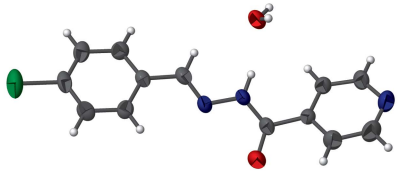
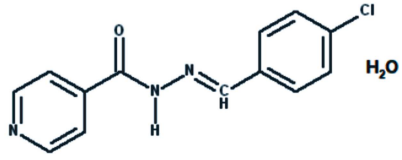
Structural data: full structural data are available from iucrdata.iucr.org

The title hydrate, $C_{13}H_{10}ClN_3O\cdot H_2O$, is the orthorhombic polymorph of the previously reported monoclinic compound [Fun *et al.* (2012). *Acta Cryst.* E**68**, o2303–o2304). In the title compound, the dihedral angle between the pyridine and benzene rings is 18.0 (2)°. In the crystal, the Schiff base molecules and water molecules are linked via O—H···O, N—H···O and O—H···N hydrogen bonds, forming a two-dimensional network parallel to (001). In addition, the Schiff base molecules are linked end-to-end by weak C—H···Cl hydrogen along the *c*-axis direction, forming an overall three-dimensional network. Weak C—H···π interactions are also observed.

3D view



Chemical scheme



Structure description

Compounds that contain an azomethine group (–HC═N–), have gained increasing attention because of their broad spectrum of biological activities (da Silva *et al.*, 2011; Kumar *et al.*, 2011). Hydrazones derived from the reactions of aldehydes with hydrazides show potential biological properties (El-Tabl *et al.*, 2008; Chen *et al.*, 2008; Álvarez *et al.*, 2008; Ventura & Martins, 2008) and have been reported to be anticancer, antifungal, antimicrobial, antiviral and antimalarial agents (Bhat *et al.*, 2015; Maccari *et al.*, 2005; Mallikarjuna *et al.*, 2009; Bekhit *et al.*, 2015). In recent years, a large number of hydrazones have been reported (*e.g.* Peng & Hou, 2008*a*; Shan *et al.*, 2008). As a part of our studies in this area, we describe herein the synthesis and crystal structure of the title compound (I).

The molecular structure of (I) is illustrated in Fig. 1. The monoclinic polymorph has already been reported (Fun *et al.*, 2012). The C7═N1 bond length of 1.273 (7) Å indicates a typical C═N double bond. The Schiff base molecule has an *E* configuration with

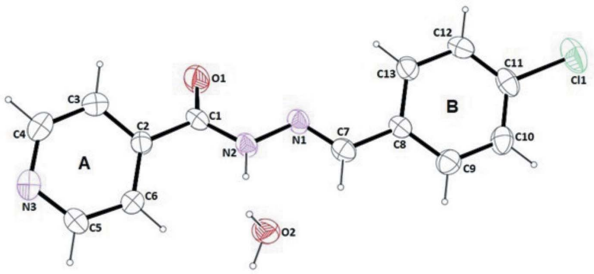


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

respect to the hydrazone bridge (C7═N1), as observed in similar compounds (Han *et al.*, 2006, Lu *et al.*, 2008, Peng & Hou 2008*b*). The dihedral angle between the benzene (A) and pyridine (B) rings is 18.0 (2)°. The bond lengths are in normal ranges.

In the crystal, the water molecules and Schiff base molecules are linked via O—H···O, N—H···O and O—H···N hydrogen bonds, forming a two-dimensional network parallel to (001) (Fig. 2). In addition, the Schiff base molecules are linked end-to-end along the *c*-axis direction by weak C—H···Cl hydrogen bonds (Fig. 3) to form an overall three-dimensional network. Weak C—H···π interactions are also observed (Table 1).

Synthesis and crystallization

A mixture of isoniazid (0.138 g, 1 mmol), 4-chlorobenzaldehyde (0.140 g, 1 mmol) and catalytic amount of ceric ammonium nitrate (2 mol %) in 5 ml of H_2O was sonicated at 60 W for 10 minutes. After completion of the reaction, as indicated by TLC, the reaction mixture was filtered and washed with distilled water. The pure title compound was obtained by recrystallization by a slow evaporation of an aqqueous alcohol solution (m.p. 455–457 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

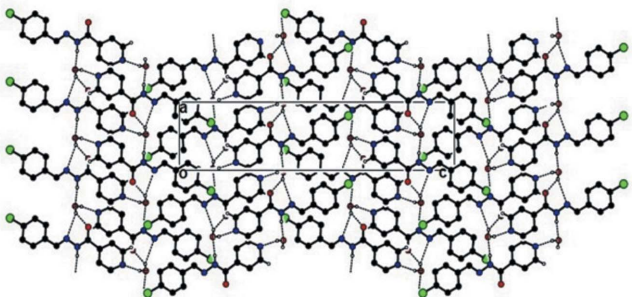


Figure 2
Part of the crystal structure with hydrogen bonds shown as dashed lines.

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

*Cg*1 and *Cg*2 are the centroids of the pyridine and benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2	0.86	2.01	2.814 (7)	156
O2—H1*O*···O1^{i}	0.80 (7)	2.19 (7)	2.907 (7)	149 (6)
O2—H2*O*···N3^{ii}	0.87 (8)	2.02 (9)	2.841 (8)	158 (8)
C4—H4···Cl1^{iii}	0.93	2.81	3.667 (7)	153
C5—H5···*Cg*1^{iv}	0.93	2.98	3.6350 (7)	129
C12—H12···*Cg*2^{v}	0.93	2.99	3.6489 (7)	129

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+3, y-\frac{1}{2}, -z-\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y+2, z-\frac{1}{2}$; (iv) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{10}ClN_3O·H_2O$
M_r	277.71
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, *b*, *c* (Å)	6.4405 (9), 7.2660 (14), 28.081 (4)
V (Å^3)	1314.1 (4)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.29
Crystal size (mm)	0.4 × 0.2 × 0.2
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Sapphire3
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min}, T_{max}	0.421, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3321, 2323, 1471
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.067, 0.148, 1.02
No. of reflections	2323
No. of parameters	181
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.25
Absolute structure	Flack *x* determined using 359 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.02 (14)

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

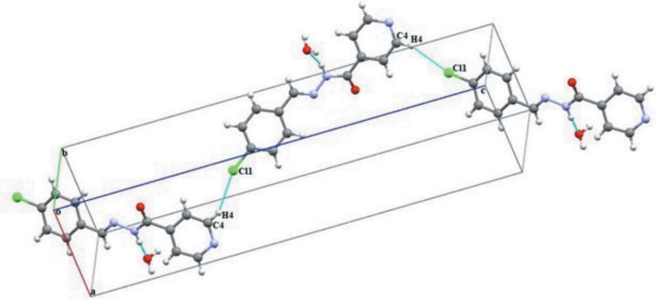


Figure 3
Part of the crystal structure showing weak C—H···Cl hydrogen bonds as dashed lines.

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full crystallographic data

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Polymorph of (*E*)-*N*′-(4-chlorobenzylidene)isonicotinohydrazide monohydrate

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(*E*)-*N*′-(4-Chlorobenzylidene)isonicotinohydrazide monohydrate

Crystal data

$C_{13}H_{10}ClN_3O·H_2O$
M_r = 277.71
Orthorhombic, $P2_12_12_1$
a = 6.4405 (9) Å
b = 7.2660 (14) Å
c = 28.081 (4) Å
V = 1314.1 (4) Å^3
Z = 4
F(000) = 576
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 945 reflections
θ = 3.8–27.0°
μ = 0.29 mm^{-1}
T = 293 K
Block, colourless
0.4 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: Enhance (Mo) X-ray Source
Detector resolution: 16.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2010)
T_{min} = 0.421, T_{max} = 1.000
3321 measured reflections
2323 independent reflections
1471 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.0°, θ_{min} = 3.6°
h = −4→7
k = −8→6
l = −29→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.148
S = 1.02
2323 reflections
181 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.2991P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.007 (2)
Absolute structure: Flack x determined using 359 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.02 (14)

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. H atoms (H1O and H2O) attached to O2 were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically and were treated as riding on their corresponding non hydrogen atoms with $U_{iso}(H) = 1.2U_{eq}(C)$ and $U_{iso}(H) = 1.2U_{eq}(N)$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.7005 (3)	0.7850 (3)	0.11474 (6)	0.0706 (7)
O1	0.8317 (7)	1.3265 (8)	−0.16937 (15)	0.0632 (16)
O2	1.5258 (8)	1.0974 (9)	−0.12165 (18)	0.0489 (13)
N1	1.0024 (8)	1.1807 (7)	−0.09043 (16)	0.0386 (13)
N2	1.1179 (7)	1.2331 (8)	−0.12955 (15)	0.0380 (14)
H2	1.251082	1.224610	−0.129120	0.046*
N3	1.3838 (9)	1.3963 (9)	−0.29400 (19)	0.0555 (17)
C1	1.0203 (10)	1.2970 (10)	−0.1680 (2)	0.0406 (16)
C2	1.1515 (9)	1.3320 (9)	−0.2110 (2)	0.0376 (16)
C3	1.0683 (10)	1.2994 (11)	−0.2556 (2)	0.0527 (19)
H3	0.933810	1.254560	−0.258866	0.063*
C4	1.1891 (12)	1.3348 (11)	−0.2953 (2)	0.062 (2)
H4	1.130033	1.314197	−0.325006	0.074*
C5	1.4597 (10)	1.4252 (10)	−0.2506 (2)	0.0480 (18)
H5	1.593842	1.471847	−0.248316	0.058*
C6	1.3554 (9)	1.3914 (10)	−0.2087 (2)	0.0428 (17)
H6	1.420595	1.408204	−0.179516	0.051*
C7	1.1053 (10)	1.1320 (9)	−0.0539 (2)	0.0384 (16)
H7	1.248760	1.146679	−0.053660	0.046*
C8	1.0029 (9)	1.0537 (9)	−0.01233 (19)	0.0335 (15)
C9	1.1064 (10)	1.0381 (10)	0.0308 (2)	0.0443 (17)
H9	1.240781	1.083767	0.033398	0.053*
C10	1.0157 (12)	0.9569 (10)	0.0699 (2)	0.0464 (18)
H10	1.087477	0.947944	0.098500	0.056*
C11	0.8155 (11)	0.8887 (9)	0.0657 (2)	0.0439 (17)
C12	0.7077 (10)	0.9055 (9)	0.0242 (2)	0.0446 (17)
H12	0.571976	0.862446	0.022230	0.054*
C13	0.7993 (10)	0.9861 (9)	−0.0151 (2)	0.0404 (16)
H13	0.725653	0.995608	−0.043441	0.048*
H1O	1.626 (11)	1.161 (10)	−0.124 (2)	0.06 (3)*
H2O	1.531 (15)	1.017 (12)	−0.144 (3)	0.10 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0999 (15)	0.0603 (13)	0.0515 (10)	−0.0130 (13)	0.0260 (11)	0.0058 (10)

O1	0.038 (3)	0.095 (5)	0.057 (3)	−0.002 (3)	0.004 (2)	0.019 (3)
O2	0.037 (3)	0.066 (4)	0.043 (3)	−0.008 (3)	0.006 (2)	−0.005 (3)
N1	0.036 (3)	0.045 (4)	0.035 (3)	0.001 (3)	0.008 (2)	0.002 (3)
N2	0.030 (2)	0.046 (4)	0.038 (3)	0.001 (3)	0.007 (2)	0.006 (3)
N3	0.061 (4)	0.068 (5)	0.037 (3)	−0.006 (4)	0.001 (3)	0.008 (3)
C1	0.034 (3)	0.045 (4)	0.043 (4)	−0.009 (4)	0.006 (3)	0.006 (3)
C2	0.033 (3)	0.045 (5)	0.034 (3)	−0.001 (3)	0.000 (3)	0.007 (3)
C3	0.043 (4)	0.067 (5)	0.047 (4)	−0.014 (4)	−0.005 (3)	0.003 (4)
C4	0.063 (5)	0.083 (7)	0.039 (4)	−0.009 (5)	−0.011 (4)	0.003 (4)
C5	0.044 (4)	0.054 (5)	0.046 (4)	−0.011 (4)	0.005 (4)	0.010 (4)
C6	0.040 (4)	0.051 (5)	0.038 (3)	−0.005 (4)	−0.003 (3)	0.003 (3)
C7	0.036 (3)	0.038 (4)	0.042 (3)	−0.001 (3)	0.008 (3)	−0.004 (3)
C8	0.035 (3)	0.031 (4)	0.035 (3)	−0.002 (3)	0.007 (3)	−0.005 (3)
C9	0.047 (4)	0.045 (4)	0.041 (4)	0.000 (3)	−0.001 (3)	−0.003 (3)
C10	0.063 (4)	0.042 (4)	0.034 (4)	0.001 (4)	0.006 (4)	−0.003 (3)
C11	0.057 (4)	0.035 (4)	0.040 (4)	0.001 (4)	0.020 (4)	−0.001 (3)
C12	0.041 (3)	0.042 (4)	0.051 (4)	−0.011 (4)	0.005 (4)	−0.004 (3)
C13	0.046 (4)	0.036 (4)	0.039 (3)	−0.004 (4)	0.000 (3)	0.003 (3)

Geometric parameters (Å, º)

Cl1—C11	1.735 (6)	C5—C6	1.375 (8)
O1—C1	1.234 (7)	C5—H5	0.9300
O2—H1O	0.80 (7)	C6—H6	0.9300
O2—H2O	0.86 (8)	C7—C8	1.455 (8)
N1—C7	1.273 (7)	C7—H7	0.9300
N1—N2	1.380 (6)	C8—C9	1.387 (8)
N2—C1	1.333 (7)	C8—C13	1.402 (8)
N2—H2	0.8600	C9—C10	1.375 (8)
N3—C5	1.331 (8)	C9—H9	0.9300
N3—C4	1.332 (8)	C10—C11	1.387 (9)
C1—C2	1.494 (8)	C10—H10	0.9300
C2—C6	1.384 (8)	C11—C12	1.364 (8)
C2—C3	1.384 (8)	C12—C13	1.380 (8)
C3—C4	1.383 (9)	C12—H12	0.9300
C3—H3	0.9300	C13—H13	0.9300
C4—H4	0.9300		
H1O—O2—H2O	108 (8)	C2—C6—H6	120.6
C7—N1—N2	116.0 (5)	N1—C7—C8	121.3 (5)
C1—N2—N1	119.1 (4)	N1—C7—H7	119.4
C1—N2—H2	120.4	C8—C7—H7	119.4
N1—N2—H2	120.4	C9—C8—C13	117.9 (6)
C5—N3—C4	115.0 (6)	C9—C8—C7	120.9 (6)
O1—C1—N2	123.4 (5)	C13—C8—C7	121.1 (5)
O1—C1—C2	120.1 (6)	C10—C9—C8	121.8 (6)
N2—C1—C2	116.5 (5)	C10—C9—H9	119.1
C6—C2—C3	117.5 (6)	C8—C9—H9	119.1

C6—C2—C1	123.6 (5)	C9—C10—C11	118.8 (7)
C3—C2—C1	118.9 (5)	C9—C10—H10	120.6
C4—C3—C2	118.7 (6)	C11—C10—H10	120.6
C4—C3—H3	120.7	C12—C11—C10	120.8 (6)
C2—C3—H3	120.7	C12—C11—Cl1	120.0 (5)
N3—C4—C3	124.8 (6)	C10—C11—Cl1	119.1 (5)
N3—C4—H4	117.6	C11—C12—C13	120.3 (6)
C3—C4—H4	117.6	C11—C12—H12	119.9
N3—C5—C6	125.1 (6)	C13—C12—H12	119.9
N3—C5—H5	117.4	C12—C13—C8	120.3 (6)
C6—C5—H5	117.4	C12—C13—H13	119.8
C5—C6—C2	118.8 (6)	C8—C13—H13	119.8
C5—C6—H6	120.6		

C7—N1—N2—C1	−175.7 (6)	C1—C2—C6—C5	−177.9 (6)
N1—N2—C1—O1	6.1 (11)	N2—N1—C7—C8	−172.8 (5)
N1—N2—C1—C2	−173.5 (6)	N1—C7—C8—C9	−165.9 (7)
O1—C1—C2—C6	146.9 (7)	N1—C7—C8—C13	16.4 (10)
N2—C1—C2—C6	−33.4 (10)	C13—C8—C9—C10	0.9 (10)
O1—C1—C2—C3	−34.8 (11)	C7—C8—C9—C10	−177.0 (6)
N2—C1—C2—C3	144.9 (7)	C8—C9—C10—C11	0.1 (11)
C6—C2—C3—C4	−2.6 (11)	C9—C10—C11—C12	−1.6 (10)
C1—C2—C3—C4	179.0 (7)	C9—C10—C11—Cl1	179.7 (5)
C5—N3—C4—C3	−0.7 (12)	C10—C11—C12—C13	2.0 (10)
C2—C3—C4—N3	1.1 (12)	Cl1—C11—C12—C13	−179.3 (5)
C4—N3—C5—C6	2.0 (11)	C11—C12—C13—C8	−0.9 (10)
N3—C5—C6—C2	−3.7 (11)	C9—C8—C13—C12	−0.5 (9)
C3—C2—C6—C5	3.8 (10)	C7—C8—C13—C12	177.3 (6)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the pyridine and benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*···O1^{i}	0.80 (7)	2.19 (7)	2.907 (7)	149 (6)
N2—H2···O2	0.86	2.01	2.814 (7)	156
O2—H2*O*···N3^{ii}	0.87 (8)	2.02 (9)	2.841 (8)	158 (8)
C4—H4···Cl1^{iii}	0.93	2.81	3.667 (7)	153
C5—H5···*Cg*1^{iv}	0.93	2.98	3.6350 (7)	129
C12—H12···*Cg*2^{v}	0.93	2.99	3.6489 (7)	129

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+3, *y*−1/2, −*z*−1/2; (iii) −*x*+3/2, −*y*+2, *z*−1/2; (iv) −*x*+2, *y*−1/2, −*z*+1/2; (v) *x*−1/2, −*y*+3/2, −*z*.