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# 3-Nitrobenzaldehyde isonicotinoylhydrazone monohydrate

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The crystal structure of the title compound, $C_{13}H_{12}N_4O_4$, contains a solvent water molecule which interacts with the organic molecules *via* intermolecular hydrogen bonds.

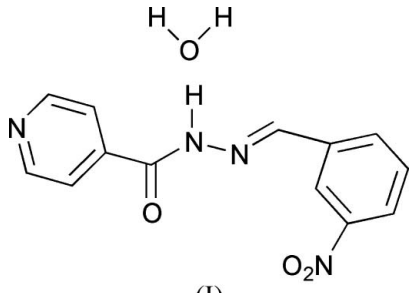
**Key indicators**

Single-crystal X-ray study
$T$ = 294 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.042
$wR$ factor = 0.127
Data-to-parameter ratio = 12.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

## Comment

Metal complexes incorporating Schiff bases have attracted much attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). Their crystal structures may provide useful information concerning their physical and chemical properties. In this context, we report here the synthesis and structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. Selected geometric parameters are listed in Table 1. The water of crystallization interacts with the organic compound molecules through hydrogen bonds (Fig. 2).

## Experimental

An anhydrous ethanol solution (50 ml) of pyridine-4-carboxylic acid hydrazide (1.37 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 3-nitrobenzaldehyde (1.51 g, 10 mmol), and the mixture was stirred at 350 K for 8 h under $N_2$, to give a yellow solution. The solvent was removed and the residue recrystallized from *N*,*N*-dimethylformamide. The product was isolated and then dried *in vacuo* to give pure (I) in 89% yield. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution of (I).

*Crystal data*

$C_{13}H_{10}N_4O_3\cdot H_2O$
$M_r$ = 288.27
Orthorhombic, *Pbca*
$a$ = 13.374 (5) Å
$b$ = 13.040 (5) Å
$c$ = 15.742 (6) Å
$V$ = 2745.5 (17) Å$^3$
$Z$ = 8
$D_x$ = 1.395 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3032 reflections
$\theta$ = 2.5–26.2°
$\mu$ = 0.11 mm$^{-1}$
$T$ = 294 (2) K
Block, yellow
0.30 × 0.20 × 0.18 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.969, $T_{max}$ = 0.981
13799 measured reflections
2430 independent reflections
1848 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 25.0°
$h = -15 \rightarrow 15$
$k = -15 \rightarrow 15$
$l = -11 \rightarrow 18$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.127
$S$ = 1.07
2430 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.4518P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C6 | 1.221 (2) | N3—C7 | 1.268 (2) |
| O2—N4 | 1.217 (2) | C5—C6 | 1.499 (2) |
| O3—N4 | 1.219 (2) | C7—C8 | 1.461 (2) |
| N2—C6 | 1.349 (2) | C8—C13 | 1.387 (2) |
| N2—N3 | 1.3823 (18) | C8—C9 | 1.391 (2) |
| | | | |
| C6—N2—N3 | 119.31 (13) | O1—C6—C5 | 121.59 (15) |
| C7—N3—N2 | 115.46 (13) | N3—C7—C8 | 121.14 (14) |
| O2—N4—O3 | 123.3 (2) | C13—C8—C7 | 120.23 (14) |
| O1—C6—N2 | 123.24 (15) | C9—C8—C7 | 121.16 (15) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O4 | 0.93 (2) | 1.96 (2) | 2.879 (2) | 170 (2) |
| O4—H4$A$···O1$^{i}$ | 0.84 (3) | 1.98 (3) | 2.812 (2) | 168 (2) |
| O4—H4$B$···N1$^{ii}$ | 0.86 (3) | 2.01 (3) | 2.876 (2) | 176 (2) |
| C1—H1···O4 | 0.93 | 2.56 | 3.282 (3) | 134 |
| C7—H7···O4 | 0.93 | 2.58 | 3.360 (2) | 142 |
| C12—H12···O3$^{iii}$ | 0.93 | 2.39 | 3.221 (3) | 148 |

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

All C-bound H atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C). The amino and water H atoms were located in a difference Fourier map and refined freely (Table 2).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

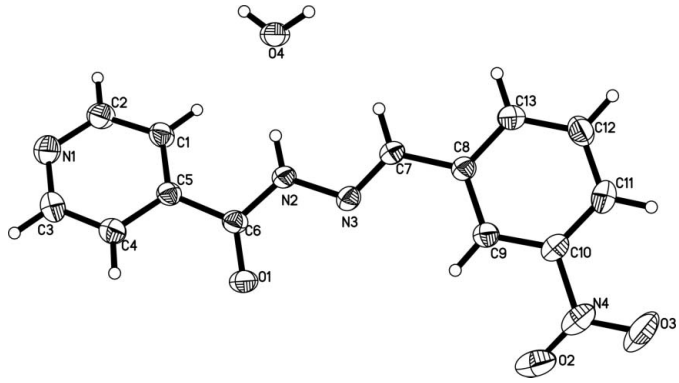



**Figure 1**
A view of the title compound, shown with 30% probability displacement ellipsoids.

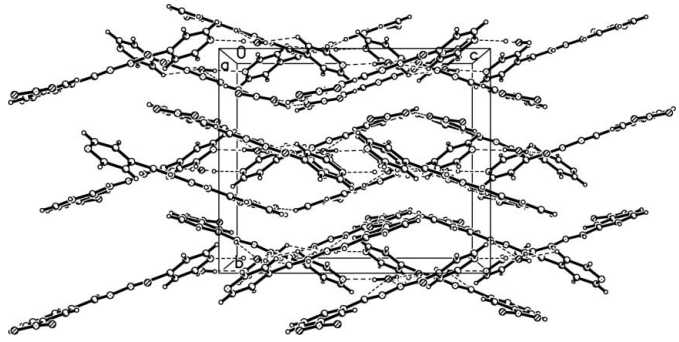



**Figure 2**
A view down the *a* axis of the crystal structure, showing the extensive intermolecular hydrogen-bonding interactions (dashed lines).

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