

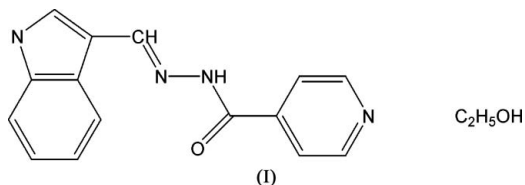
Zuo-Liang Jing,* Wen-Wen
Cheng, Xin Chen and Yu MingCollege of Sciences, Tianjin University of
Science and Technology, Tianjin 300222,
People's Republic of China

Correspondence e-mail: jzl74@tust.edu.cn

Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.034
 wR factor = 0.101
Data-to-parameter ratio = 7.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2'-(1*H*-Indol-3-ylmethylene)isonicotino-
hydrazide ethanol solvateIn the crystal structure of the title compound, $\text{C}_{15}\text{H}_{12}\text{N}_4\text{O} \cdot \text{C}_2\text{H}_6\text{O}$, molecules are linked *via* weak intermolecular $\text{N}-\text{H} \cdots \text{N}$, $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds, forming a two-dimensional network.Received 24 February 2006
Accepted 7 March 2006

Comment

Metal complexes based on 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). As part of an investigation of the coordination properties of Schiff bases functioning as ligands (Yu *et al.*, 2005; Deng *et al.*, 2005; Jing *et al.*, 2005; Guo *et al.*, 2006), we report the synthesis and structure of the title compound, (I).The 4-pyridyl (C1–C6/N1) and 1*H*-indole-3-carbaldehyde (C7–C15/N4) units are planar, with r.m.s. deviations of 0.0117 (2) and 0.0140 (5) Å, respectively (Fig. 1). The dihedral angle between these planes is 43.60 (6)°. Intermolecular $\text{N}-\text{H} \cdots \text{N}$, $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds (Table 2) form a two-dimensional network (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 1*H*-indole-3-carbaldehyde (1.46 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of pyridine-4-carboxylic acid hydrazide (1.37 g, 10 mmol) and the mixture was stirred at 330 K for 6 h under N_2 , whereupon a red solution appeared. The solvent was removed and the residue was recrystallized from anhydrous ethanol. The product was isolated and then dried *in vacuo* to give pure (I) in 86% yield. Red single crystals suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution.

Crystal data

 $\text{C}_{15}\text{H}_{12}\text{N}_4\text{O} \cdot \text{C}_2\text{H}_6\text{O}$
 $M_r = 310.35$
Orthorhombic, $P2_12_12_1$
 $a = 9.6080$ (14) Å
 $b = 10.0047$ (15) Å
 $c = 16.791$ (3) Å
 $V = 1614.1$ (4) Å³
 $Z = 4$
 $D_x = 1.277$ Mg m⁻³Mo $K\alpha$ radiation
Cell parameters from 4354
reflections
 $\theta = 2.4$ – 24.6°
 $\mu = 0.09$ mm⁻¹
 $T = 294$ (2) K
Block, red
 $0.38 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	1651 independent reflections
φ and ω scans	1554 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.023$
$T_{\text{min}} = 0.752$, $T_{\text{max}} = 0.983$	$\theta_{\text{max}} = 25.0^\circ$
8779 measured reflections	$h = -11 \rightarrow 11$
	$k = -11 \rightarrow 9$
	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.3045P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.101$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$
1651 reflections	$\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$
219 parameters	Extinction correction: <i>SHELXL97</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.022 (3)

Table 1

Selected geometric parameters (\AA , $^\circ$).

O1—C6	1.236 (3)	N4—C14	1.375 (3)
N2—C6	1.330 (3)	C5—C6	1.495 (3)
N2—N3	1.392 (3)	C7—C8	1.437 (3)
N3—C7	1.278 (3)	C8—C9	1.445 (3)
N4—C15	1.347 (3)		
C6—N2—N3	120.33 (19)	C15—C8—C7	123.3 (2)
C7—N3—N2	113.29 (18)	O1—C6—N2	124.7 (2)
C7—C8—C9	130.5 (2)	O1—C6—C5	120.6 (2)
C15—N4—C14	109.56 (19)	N2—C6—C5	114.64 (19)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2B \cdots N1 ⁱ	0.91 (3)	2.12 (3)	3.015 (3)	169 (2)
N4—H4A \cdots O1 ⁱⁱⁱ	0.78 (3)	2.15 (3)	2.917 (3)	168 (3)
O2—H2A \cdots O1 ⁱⁱⁱ	0.82	1.96	2.778 (3)	179

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

N-bound H atoms were located in a difference Fourier map and refined freely. C- and O-bound H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.93–0.97 \AA and O—H = 0.82 \AA , and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C and O})$. In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

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, 1999); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1999). *SHELXTL* (Version 5.10), *SMART* (Version 5.0) and *SAINT* (Version 4.0). Bruker AXS Inc., Madison, Wisconsin, USA.

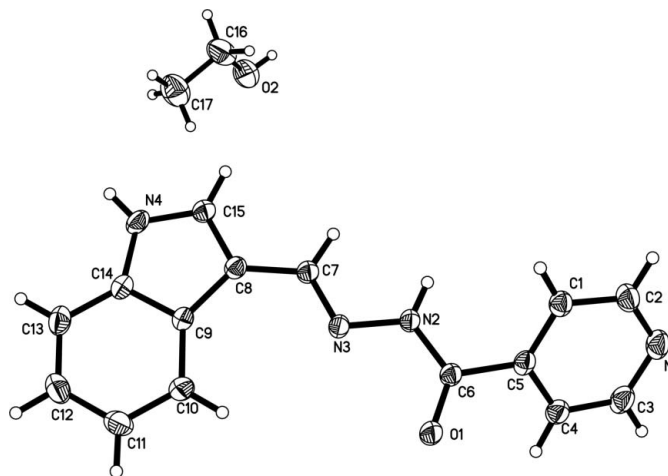


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

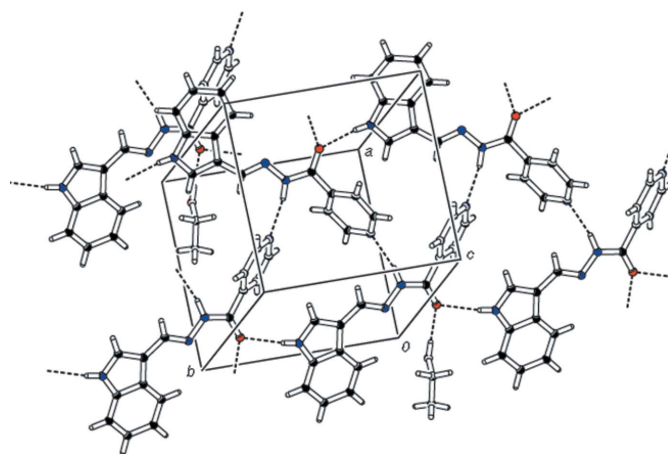


Figure 2

Packing view of (I), showing the intermolecular hydrogen bonds (dashed lines).

- Deng, Q.-L., Yu, M., Chen, X., Diao, C.-H., Jing, Z.-L. & Fan, Z. (2005). *Acta Cryst.* **E61**, o2545–o2546.
- Guo, M.-J., Sun, J.-C., Jing, Z.-L., Yu, M. & Chen, X. (2006). *Acta Cryst.* **E62**, o820–o821.
- Jing, Z.-L., Fan, Z., Yu, M., Chen, X. & Deng, Q.-L. (2005). *Acta Cryst.* **E61**, o3208–o3209.
- Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.
- Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Yu, M., Chen, X., & Jing, Z.-L. (2005). *Acta Cryst.* **E61**, o1345–o1346.