Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Oxo-2,3-dihydro-1*H*-indol-3-one nicotinoylhydrazone

Hapipah M. Ali, Siti Nadiah Abdul Halim, Wan Jefri Basirun and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.109
Data-to-parameter ratio = 12.0

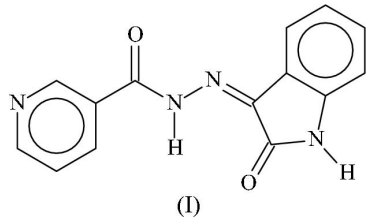
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 25 February 2005
Accepted 3 March 2005
Online 11 March 2005

In the title structure, $C_{14}H_{10}N_4O_2$, the pyridyl ring is twisted with respect to the central —C(=O)—NH—N= fragment by 17.7 (1)°, whereas the indole fused-ring system is almost coplanar with this fragment. Molecules are linked into a linear chain motif by N—H···O hydrogen bonds.

Comment

The crystal structure of isatin 2-picolylhydrazone, (II), has been determined as part of a report on the biological activity of its transition metal derivatives. The molecule adopts a nearly planar conformation, the planar nature being conducive to *N*,*N*′,*O*-chelation in the deprotonated compound (Rodríguez-Argüelles *et al.*, 2004).



(I)

The isomeric title molecule, (I) (Fig. 1), adopts a somewhat non-planar conformation. The pyridyl ring is twisted by 17.7 (1)° with respect to the central —C(=O)—NH—N= fragment, while the indole fused-ring system is nearly coplanar with this fragment [4.1 (1)°]. The bond distances and angles in (I) and (II) are the same within experimental error. In the crystal structure of (I), molecules are linked into a linear chain by N—H···O hydrogen bonds (Table 1 and Fig. 2). Transition metal derivatives of the title compound have been reported, but these have not been crystallographically verified (Srivastava *et al.*, 2000).

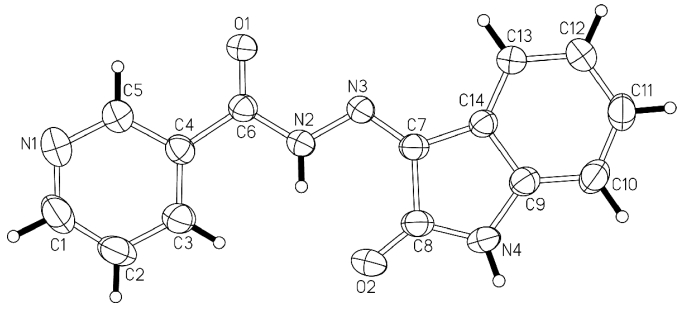


Figure 1
ORTEPII plot (Johnson, 1976) of the title molecule. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

Experimental

Isatin (0.50 g, 3.39 mmol) and nicotinoyl hydrazide (4.66 g, 3.39 mmol) were dissolved in ethanol (30 ml); the solution was heated under reflux for 2 h. The orange solid that was isolated when the solution was cooled was collected and recrystallized from dimethylformamide to afford block crystals.

Crystal data

$C_{14}H_{10}N_4O_2$
$M_r = 266.26$
Monoclinic, $P2_1/c$
$a = 8.9066$ (5) Å
$b = 11.7021$ (6) Å
$c = 11.7768$ (6) Å
$\beta = 97.097$ (1)°
$V = 1218.0$ (1) Å^3
$Z = 4$
$D_x = 1.452$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5073 reflections
$\theta = 2.3$–27.0°
$\mu = 0.10$ mm^{-1}
$T = 295$ (2) K
Block, orange
0.37 × 0.35 × 0.32 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
10102 measured reflections
2643 independent reflections
2149 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.0°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.109$
$S = 1.00$
2643 reflections
221 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 0.2785P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2n···O2	0.86 (1)	2.00 (1)	2.711 (2)	139 (2)
N4—H4n···O1^{i}	0.86 (1)	2.15 (1)	2.941 (2)	153 (2)

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

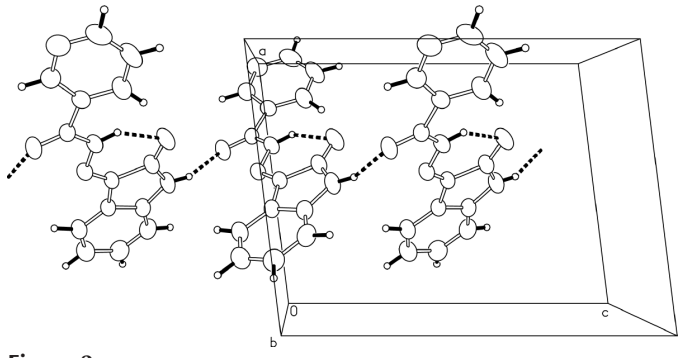


Figure 2
ORTEPII plot (Johnson, 1976) of the hydrogen-bonded chain. Hydrogen bonds are indicated by dashed lines.

The positional parameters of all H atoms were refined with restraints of N—H = 0.86 (1) Å and C—H = 0.95 (1) Å; the isotropic displacement parameters were refined without restraint.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the Ministry of Science, Technology and the Environment for supporting this study (grant No. IPRA 33-02-03-3055). We acknowledge Mr Xiao-Long Feng of Sun Yat-Sen University for the diffraction measurements.

References

Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rodríguez-Argüelles, M. C., Ferrari, M. B., Bisceglie, F., Pelizzi, C., Pelosi, G., Pinell, S. & Sassi, M. (2004). *J. Inorg. Biochem.* **98**, 313–321.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Srivastava, A. K., Pandey, O. P. & Sengupta, S. K. (2000). *Synth. React. Inorg. Met. Org. Chem.* **30**, 1405–1416.