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2,3-Dihydro-1*H*-indole-2,3-dione 3-isonicotinoylhydrazone

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In the title compound, $C_{14}H_{10}N_4O_2$, the pyridine ring and the isatin unit (indoline-2,3-dione) are nearly coplanar, the dihedral angle being 3.79 (11)°. Inter- and intramolecular N—H···O hydrogen bonding and weak intermolecular C—H···O hydrogen bonding occur in the crystal structure.

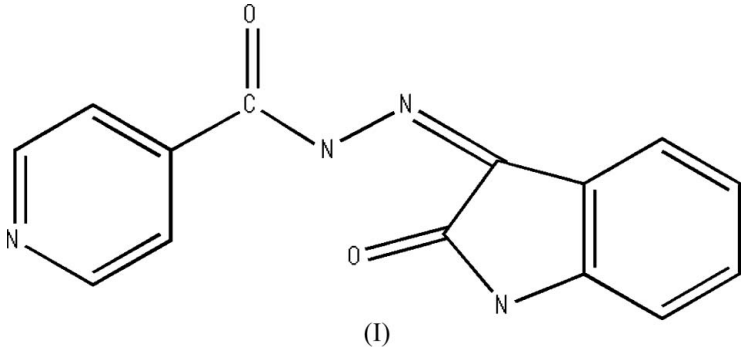
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.026
wR factor = 0.073
Data-to-parameter ratio = 6.5

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

Comment

Isatin, indoline-2,3-dione, has recently been found to be an endogenous polyfunctional heterocyclic compound, exhibiting biological activity in mammals (Somogyi, 2001). Several metal complexes with isatin isonicotinoylhydrazone have been prepared (Hassaan, 1997). We report here the crystal structure of isatin isonicotinoylhydrazone, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The pyridine ring and the isatin unit are nearly coplanar, the dihedral angle being 3.79 (11)°. The bond distances (Table 1) show electron delocalization within the hydrazone group. Inter- and intramolecular N—H···O hydrogen bonding and weak intermolecular C—H···O hydrogen bonding occur in the crystal structure of (I) (Table 2).

Experimental

The title compound was prepared according to the literature method of Hassaan (1997). Single crystals of (I) were obtained by slow evaporation of the filtrate of the resulting mixture at room temperature.

Crystal data

$C_{14}H_{10}N_4O_2$
M_r = 266.26
Orthorhombic, $Pna2_1$
a = 8.007 (5) Å
b = 28.561 (16) Å
c = 5.266 (3) Å
V = 1204.2 (12) Å^3
Z = 4
D_x = 1.469 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, red
0.28 × 0.22 × 0.18 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
6229 measured reflections
1191 independent reflections
1109 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.073$
$S = 1.06$
1191 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.107P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.09$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.013 (2)

Table 1
Selected bond lengths (Å).

O1—C8	1.227 (2)	N2—N3	1.369 (2)
O2—C9	1.216 (3)	N3—C9	1.351 (3)
N2—C7	1.289 (3)	C9—C10	1.504 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.12	2.861 (3)	144
N3—H3A···O1	0.86	2.00	2.695 (3)	137
C5—H5···O1^{ii}	0.93	2.36	3.283 (3)	172

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

H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined in riding mode, with U_{iso}(H) = $1.2U_{eq}$(C,N). In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

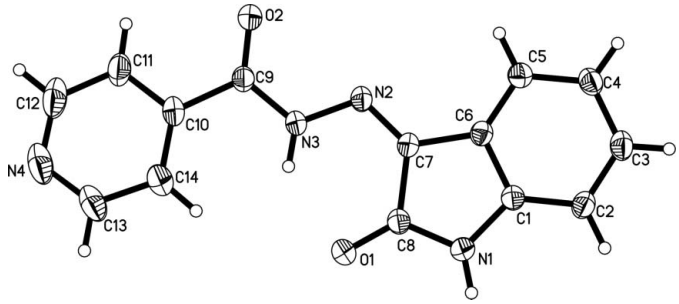


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

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