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# 1,5-Dimethyl-4-[(2-oxo-2,3-dihydro-1*H*-indol-3-ylidene)amino]-2-phenyl-1*H*-pyrazol-3(2*H*)-one monohydrate

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**Key indicators**

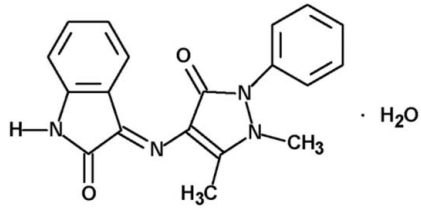
Single-crystal X-ray study
*T* = 291 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.067
*wR* factor = 0.149
Data-to-parameter ratio = 11.5

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

Molecules of the title compound, $C_{19}H_{16}N_4O_2\cdot H_2O$, are linked into a one-dimensional ladder structure by a combination of intermolecular O—H···O and N—H···O hydrogen bonds.

## Comment

Isatin (indol-2,3-dione) (Sharma *et al.*, 2002) and antipyrine (2,3-dimethyl-1-phenyl-5-pyrazolone) (Yadav *et al.*, 2003) have been long known for their wide spectrum of biological activities. In continuation of our studies on isatin derivatives, we now report the synthesis and crystal structure of the title compound, (I).




(I)

In (I) (Fig. 1), the mean planes of the indole and phenyl ring systems are twisted out of the pyrazole ring mean plane by 56.7 (3) and 52.8 (3)°, respectively. All the geometrical parameters for (I) lie within their expected ranges, and are in agreement with the corresponding values reported by Sun *et al.* (2006, 2007).

The water molecule plays an important role in the structure of (I), owing to its participation in hydrogen bonding (Table 1), acting as both a donor for O—H···O bonds and an acceptor

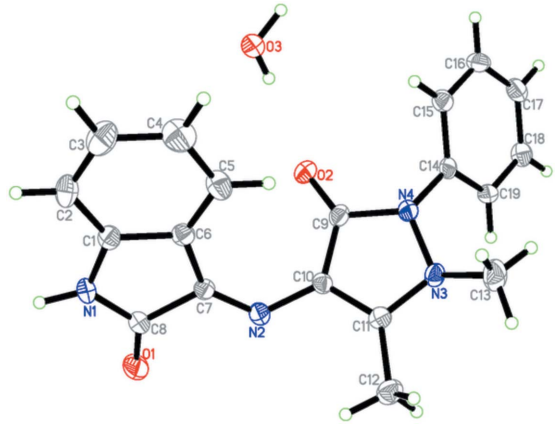



**Figure 1**
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

for an N—H···O bond. Together, the hydrogen bonds give rise to one-dimensional molecular chains (Fig. 2) propagating in [010].

## Experimental

A mixture of isatin (1 mmol) and 4-aminoantipyrine (1 mmol) in ethanol (25 ml) was refluxed for 5 h, and then cooled to room temperature. The precipitate was filtered off and dried. The crude product was recrystallized from ethanol, yielding the title compound in 78% yield (m.p. 499–501 K). Analysis calculated for $C_{19}H_{18}N_4O_3$: C 65.13, H 5.18, N 15.99%; found: C 65.05, H 5.36, N 15.73%. Red prisms of (I) were obtained by slow evaporation of an ethanol solution at room temperature.

*Crystal data*

$C_{19}H_{16}N_4O_2\cdot H_2O$
$M_r$ = 350.37
Monoclinic, $C2/c$
$a$ = 17.587 (4) Å
$b$ = 7.2102 (14) Å
$c$ = 28.973 (6) Å
$\beta$ = 106.00 (3)°
$V$ = 3531.8 (12) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 291 (2) K
0.20 × 0.18 × 0.17 mm

*Data collection*

Rigaku R-AXIS-IV diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.982, $T_{max}$ = 0.985
4696 measured reflections
2852 independent reflections
1876 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.062

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.149
$S$ = 1.05
2852 reflections
248 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$B$···O3$^{i}$ | 0.93 (4) | 1.87 (4) | 2.790 (4) | 171 (4) |
| O3—H3$F$···O1$^{ii}$ | 0.92 (5) | 1.91 (5) | 2.796 (4) | 163 (5) |
| O3—H3$E$···O2$^{iii}$ | 0.75 (5) | 2.05 (5) | 2.780 (5) | 165 (6) |

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

All H atoms were initially located in a difference Fourier map. The C-bound H atoms were then constrained to an ideal geometry, with C—H = 0.93–0.96 Å, and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C). The positions and $U_{iso}$ values of the H atoms bonded to N and O atoms were refined freely.

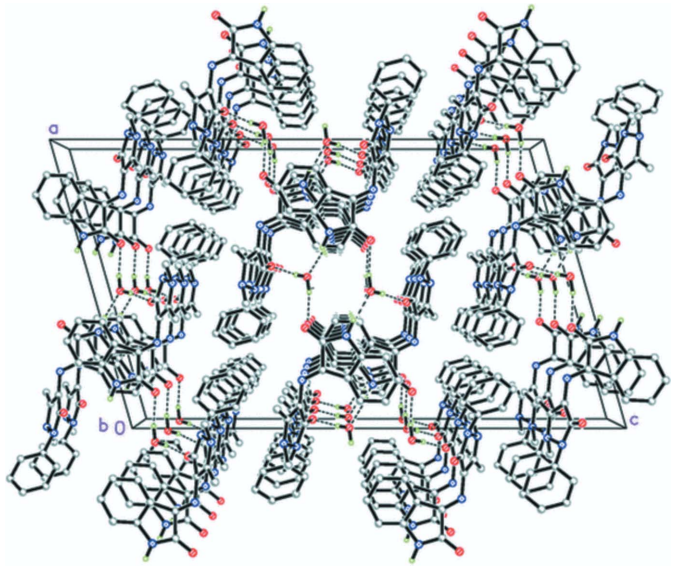



**Figure 2**
A packing diagram for (I), viewed down the $b$ axis. Dashed lines indicate hydrogen bonds.

Data collection: *R-AXIS* (Rigaku,1996); cell refinement: *R-AXIS*; data reduction: *R-AXIS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1999); software used to prepare material for publication: *TEXSAN*.

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