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4-(1*H*-Indol-3-ylmethyleneamino)-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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In the crystal structure of the title compound, $C_{20}H_{18}N_4O$, the molecules are linked *via* weak intermolecular N—H···O hydrogen bonds, forming an extended supramolecule.

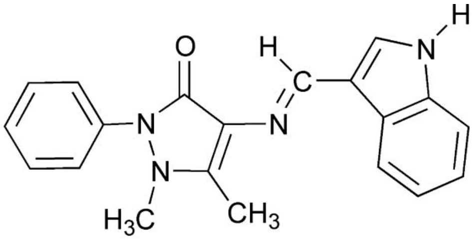
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.074
Data-to-parameter ratio = 7.9

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

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 into 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).



(I)

In the molecular structure of (I) (Fig. 1), the expected geometric parameters are observed. The central chromophore (C10–C12/N3/N4) is planar, with an r.m.s. deviation for the fitted atoms of 0.036 (2) Å, as are the 1*H*-indole-3-carbaldehyde group (C1–C8/N1), with an r.m.s. deviation of 0.0083 (5) Å, and the phenyl group (C15–C20), with an r.m.s. deviation of 0.0034 (6) Å. The dihedral angles formed between these last two planes and that through the C10–C12/N3/N4 ring are 6.29 (9) and 60.98 (6)°, respectively. The C1–C8/N1 and C15–C20 groups are inclined at 67.15 (6)°. There are intermolecular N—H···O hydrogen bonds (Table 1) and the molecules associate in a zigzag pattern along the *b* axis, forming a supramolecular structure, as illustrated in 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 4-amino-1,5-dimethyl-2-phenyl-1,2-dihydropyrazol-3-one (2.03 g, 10 mmol) and the mixture was stirred at 330 K for 6 h under N_2, whereupon a yellow solution appeared. The solvent was removed and the residue recrystallized from anhydrous ethanol. The product was isolated and then dried *in vacuo* to give pure (I) in 83% yield. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution of (I).

Crystal data

$C_{20}H_{18}N_4O$
$M_r = 330.38$
Orthorhombic, $P2_12_12_1$
$a = 6.857$ (3) Å
$b = 15.729$ (8) Å
$c = 16.436$ (8) Å
$V = 1772.5$ (15) Å^3
$Z = 4$
$D_x = 1.238$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 294$ (2) K
Block, yellow
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.972$, $T_{\max} = 0.984$
9604 measured reflections
1822 independent reflections
1583 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.074$
$S = 1.06$
1822 reflections
232 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 0.0654P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.10$ e Å^{-3}
$\Delta\rho_{\min} = -0.08$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0116 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1$^{\rm i}$	0.89 (3)	1.92 (3)	2.794 (2)	166 (2)

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

The N-bound H atom was located in a difference Fourier map and its position was refined freely; $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm N})$. C-bound H atoms were included in calculated positions and refined using the riding-model approximation; C—H = 0.93 (aromatic) and 0.96 Å (methyl), with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for aromatic H and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H. In the absence of significant anomalous scattering 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, 1997); software used to prepare material for publication: *SHELXTL*.

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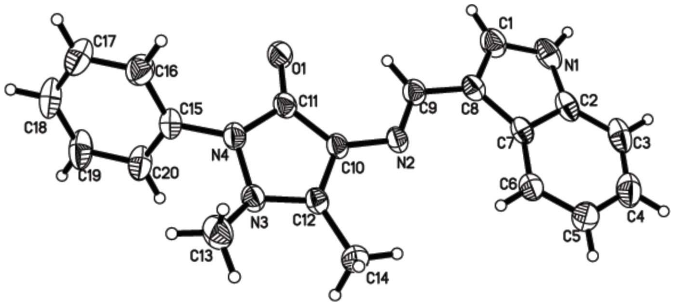

Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

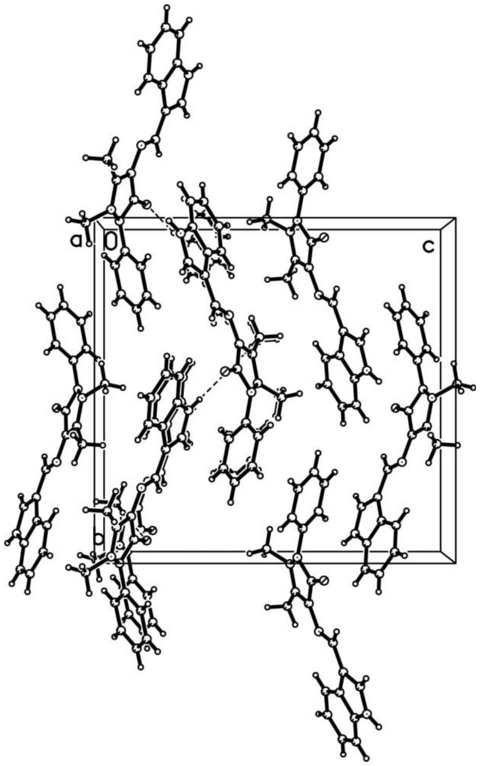

Figure 2
A view down the b axis showing the intermolecular hydrogen-bonding interaction (dashed line).

References

Bruker (1997). *SHELXTL*. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.

Deng, Q.-L., Yu, M., Chen, X., Diao, C.-H., Jing, Z.-L. & Fan, Z. (2005). *Acta Cryst.* E**61**, o2545–o2546.

Guo, M.-J., Sun, J.-C., Jing, Z.-L., Yu, M. & Chen, X. (2006). *Acta Cryst.* E**62**, o820–o821.

Jing, Z.-L., Fan, Z., Yu, M., Chen, X. & Deng, Q.-L. (2005). *Acta Cryst.* E**61**, 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.* E**61**, o1345–o1346.

Acta Cryst. (2007). E**63**, o418–o419 Zhou *et al.* • $C_{20}H_{18}N_4O$ **o419**