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1,5-Dimethyl-2-phenyl-4-[(1*H*-pyrrol-2-ylmethylene)amino]pyrazol-3(2*H*)-one

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Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.121
Data-to-parameter ratio = 17.0

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

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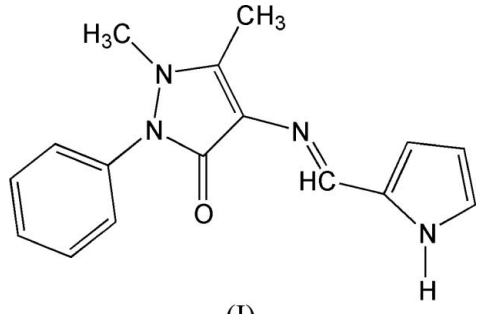
In the crystal structure of the title compound, $C_{16}H_{16}N_4O$, the molecules are linked *via* weak intermolecular N—H···O hydrogen bonds, forming an extended supramolecular arrangement.

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, Fan *et al.*, 2005; Guo, Sun *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 chomophore (atoms C1–C3/N1/N2) is planar, with an r.m.s. deviation for the fitted atoms of 0.0159 (2) Å, as are the 1*H*-pyrrole-2-carbaldehyde group (C11–C14/N4), with an r.m.s. deviation of 0.0017 (3) Å, and the phenyl ring (C4–C9), with an r.m.s. deviation of 0.0063 (6) Å. The dihedral angles formed between these last two planes and that through the C1–C3/N1/N2 ring are 27.66 (6) and 62.54 (5)°, respectively. The C11–C14/N4 and C4–C9 groups are inclined at an angle of 84.11 (4)°. There are intermolecular N—H···O hydrogen bonds (Table 1) and the molecules associate in a zigzag pattern along the *a* axis, forming a supramolecular structure, as illustrated in Fig. 2.

Experimental

An anhydrous ethanol solution (50 ml) of 1*H*-pyrrole-2-carbaldehyde (0.95 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3(2*H*)-one (2.03 g, 10 mmol) and the mixture was stirred at 350 K for 6 h under N_2, whereupon a colourless solution appeared. The solvent was removed

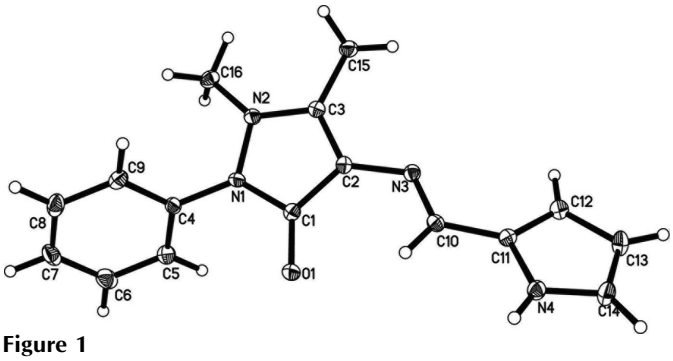


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

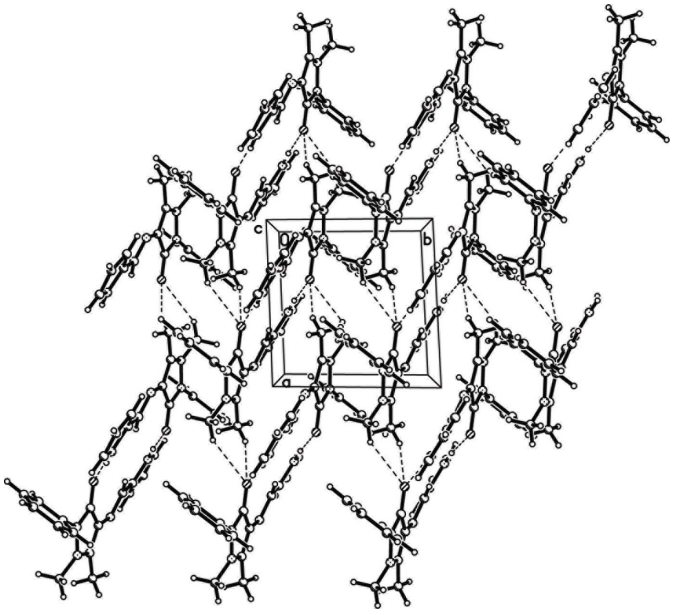


Figure 2
A view down the *c* axis of a portion of the crystal structure of (I), showing extensive intermolecular hydrogen-bonding interactions (dashed lines).

and the residue recrystallized from anhydrous ethanol. The product was isolated and then dried *in vacuo* to give pure (I) in 75% yield. Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution of (I).

Crystal data

$C_{16}H_{16}N_4O$
M_r = 280.33
Triclinic, $P\overline{1}$
a = 7.3142 (4) Å
b = 7.3170 (3) Å
c = 13.5485 (6) Å
α = 80.791 (7)°
β = 82.639 (7)°
γ = 86.330 (7)°
V = 709.14 (6) Å^3
Z = 2
D_x = 1.313 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 113 (2) K
Prism, colourless
0.20 × 0.16 × 0.14 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.983, T_{max} = 0.988
8890 measured reflections
3346 independent reflections
2367 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.121
S = 1.06
3346 reflections
197 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.038 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O1^{i}	0.862 (17)	1.959 (18)	2.8117 (16)	170.3 (17)

Symmetry code: (i) $-x+1, -y, -z+1$.

The N-bound H atom was located in a difference Fourier map and its position was refined freely. C-bound H atoms were included in calculated positions and refined using the riding-model approximation; C—H = 0.95 (aromatic) and 0.98 Å (methyl), with U_{iso}(H) = 1.2U_{eq}(C) for aromatic and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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