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1,5-Dimethyl-4-(3-nitrobenzylideneamino)-2-phenylpyrazolidin-3-one

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The title compound, $C_{18}H_{16}N_4O_3$, was prepared by the reaction of 3-nitrobenzaldehyde and 4-amino-1,5-dimethyl-2-phenyl-pyrazol-3-one. The crystal structure displays an intramolecular C—H···O hydrogen bond, which may stabilize the conformation of the molecule, as well as intermolecular C—H···O hydrogen bonds.

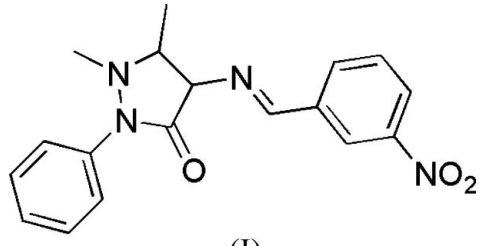
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.062
wR factor = 0.225
Data-to-parameter ratio = 12.6

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

Comment

The syntheses and structures of Schiff bases have attracted much attention, because their metal complexes have been studied extensively as model compounds of biologically active compounds (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of this investigation, we report here the synthesis and crystal structure of the title compound, (I).



(I)

A view of the molecular structure of (I) is shown in Fig. 1. The pyrazolidinone group C8–C10/N1–N3/O3 is planar, with an r.m.s. deviation for the fitted atoms of 0.0409 Å. This plane makes a dihedral angle of 48.55 (11)° with the phenyl ring (C13–C18) and a dihedral angle of 10.07 (11) ° with the nitrobenzene ring (C1–C7/N4).

The intramolecular C—H···O hydrogen bond (Table 1), may help to stabilize the observed conformation of the molecule. In the crystal structure, the molecules are associated *via* weak C—H···O intermolecular hydrogen bonds (Table 1) to form a layer structure (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 3-nitrobenzaldehyde (1.51 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen, whereupon a yellow precipitate was formed. The product was isolated and recrystallized from ethanol, and then dried *in vacuo* to give pure (I) in 83% yield. Bright-yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

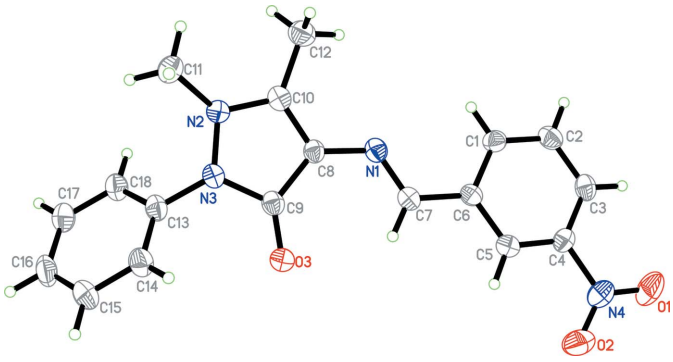


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 30% probability level.

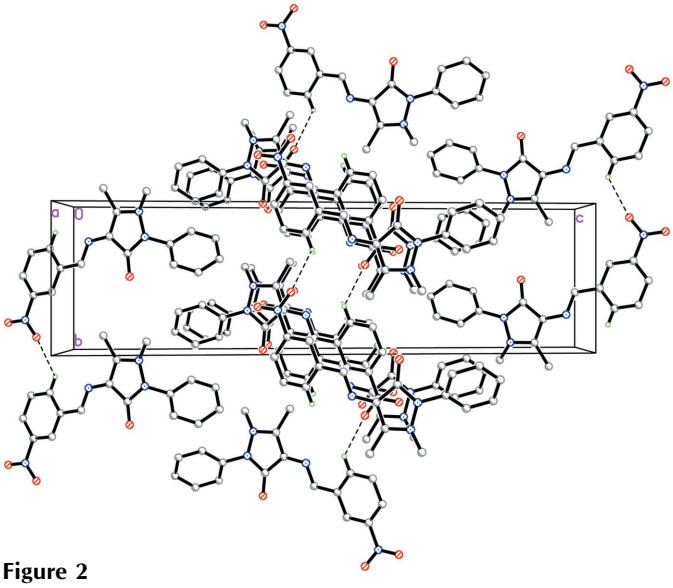


Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines) in the crystal structure of (I). H atoms not involved in hydrogen bonds have been omitted.

Crystal data

$C_{18}H_{16}N_4O_3$
M_r = 336.35
Monoclinic, $P2_1/c$
a = 7.645 (11) Å
b = 7.839 (11) Å
c = 28.24 (4) Å
β = 96.349 (19)°
V = 1682 (4) Å^3
Z = 4
D_x = 1.328 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1975 reflections
θ = 2.7–25.8°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, yellow
0.32 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.962, T_{max} = 0.985
8161 measured reflections
2891 independent reflections
1817 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 25.0°
$h = -6 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.225
S = 1.00
2891 reflections
229 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1519P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.008 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O3	0.93	2.45	3.094 (5)	126
C1—H1···O2^{i}	0.93	2.44	3.125 (6)	131

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

H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl CH_3.

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, 1999); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1999). *SHELXTL* (Version 5.10), *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.
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.