Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[(4-Methoxybenzylidene)amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

Zuo-Liang Jing,* Min-Jie Guo, Xin Chen and Yu Ming

College of Sciences, Tianjin University of Science and Technology, Tianjin 300222, People's Republic of China

Correspondence e-mail: jzl74@tust.edu.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.120
Data-to-parameter ratio = 18.0

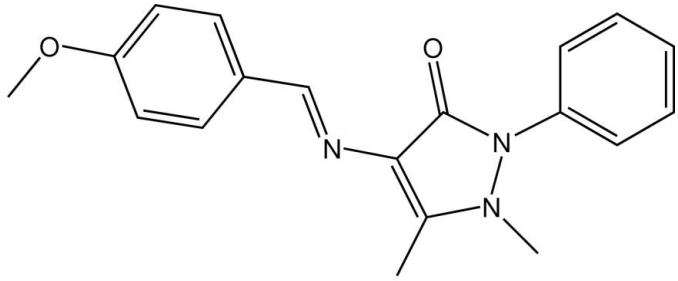
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 23 November 2005
Accepted 14 December 2005
Online 21 December 2005

The crystal structure of the title compound, $C_{19}H_{19}N_3O_2$, shows the molecule to be essentially planar with the exception of the terminal phenyl group. Molecules are associated *via* intermolecular C—H···O hydrogen bonds.

Comment

Metal complexes of Schiff bases have attracted much attention because they can be utilized as model compounds for the active centres in various enzymes and proteins (Kahwa *et al.*, 1986; Santos *et al.*, 2001). Important to the understanding of the coordination potential of these ligands is a knowledge of the ligand structure. Accordingly, the synthesis and crystal structures of Schiff base ligands derived from 4-aminoantipyrine, such as thenoyltrifluoroacetone (Yu *et al.*, 2002), 4-hydroxy-3-methoxybenzaldehyde (Diao *et al.*, 2005) and 2,4-dichlorobenzaldehyde (Jing *et al.*, 2005), have been reported.



(I)

In the molecular structure of the related title compound, (I) (Fig. 1), the expected geometric parameters are observed (Table 1). The central chromophore containing the C9–C11/N1–N3/O2 atoms is planar, with an r.m.s. deviation for fitted atoms of 0.038 (2) Å; the 4-methoxybenzylidene group (C1–C8/O1) is also planar, with an r.m.s. deviation of 0.027 (5) Å. The dihedral angles formed between these planes and that

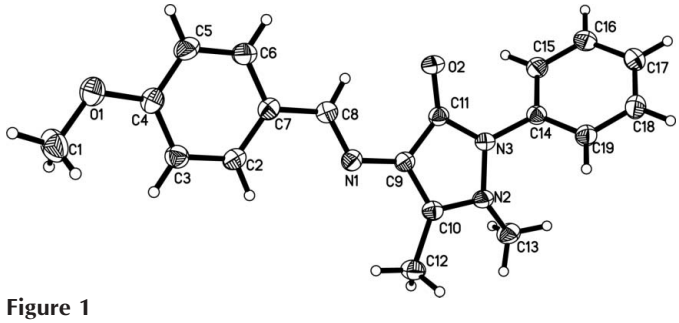


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

through the C14–C19 phenyl ring are 48.24 (5) and 9.40 (6)°, respectively. Intramolecular C—H···O hydrogen bonding stabilizes the molecular conformation, while intermolecular C—H···O hydrogen bonding stabilizes the crystal structure; geometric details are given in Table 2. The molecules associate in a zigzag pattern along the *c* axis, forming a supramolecular structure, as illustrated in Fig. 2.

Experimental

An anhydrous ethanol solution of 4-methoxybenzaldehyde (1.36 g, 10 mmol) was added to an anhydrous ethanol solution of 4-amino-1,5-dimethyl-2-phenyl-1,2-dihydropyrazol-3-one (2.03 g, 10 mmol) and the mixture was stirred at 350 K for 8 h under N_2, whereupon a yellow solution appeared. The solvent was removed and the residue recrystallized from *N*,*N*-dimethylformamide. The product was isolated and then dried *in vacuo* to give pure (I) in 79% yield. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution of (I).

Crystal data

$C_{19}H_{19}N_3O_2$
M_r = 321.37
Monoclinic, $P2_1/c$
a = 7.1407 (10) Å
b = 24.864 (3) Å
c = 9.4733 (13) Å
β = 96.700 (2)°
V = 1670.4 (4) Å^3
Z = 4
D_x = 1.278 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2518 reflections
θ = 2.3–23.6°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, yellow
0.20 × 0.16 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.988
11145 measured reflections
3949 independent reflections
2677 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.8°
$h = -9 \rightarrow 8$
$k = -31 \rightarrow 32$
$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.04
3949 reflections
220 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 0.1906P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.422 (2)	N2—C10	1.3589 (18)
O1—C4	1.3684 (18)	N2—C13	1.4620 (17)
O2—C11	1.2336 (16)	N3—C11	1.4065 (17)
N1—C8	1.2754 (18)	N3—C14	1.4181 (17)
N1—C9	1.3920 (17)	C7—C8	1.460 (2)
N2—N3	1.4040 (15)	C9—C11	1.436 (2)
C1—O1—C4	117.94 (13)	N2—N3—C14	120.21 (11)
C8—N1—C9	120.85 (13)	C11—N3—C14	122.99 (11)
N3—N2—C10	107.12 (10)	N1—C8—C7	121.58 (14)
N3—N2—C13	117.60 (11)	O2—C11—N3	122.87 (13)
C10—N2—C13	123.72 (12)	O2—C11—C9	131.99 (13)
N2—N3—C11	108.88 (11)		

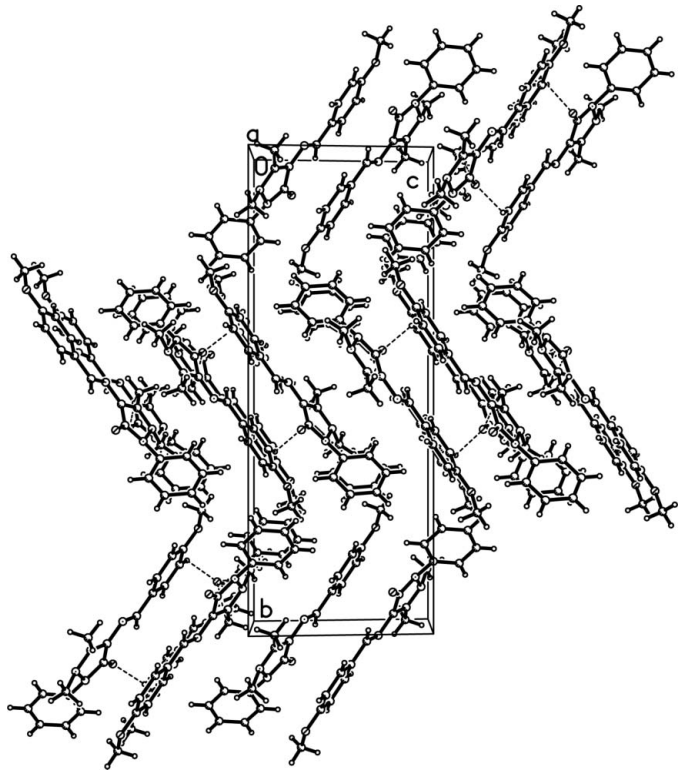


Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines) in (I).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2	0.93	2.34	3.0310 (18)	131
C5—H5···O2^{i}	0.93	2.56	3.2838 (19)	135
C12—H12*A*···O2^{ii}	0.96	2.43	3.3815 (19)	172

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $x+1, y, z$.

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

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*.

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.
Diao, C.-H., Fan, Z., Yu, M., Chen, X., Jing, Z.-L. & Deng, Q.-L. (2005). *Acta Cryst.* E**61**, o2322–o2323.
Jing, Z.-L., Yu, M., Chen, X. & Deng, Q.-L. (2005). *Acta Cryst.* E**61**, o3359–o3360.

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., Wang, J.-L. & Miao, F.-M. (2002). *Acta Cryst.* E**58**, o1182–o1184.