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(*E*)-1,5-Dimethyl-4-{2-[2-(2-nitrophenoxy)-ethoxy]benzylideneamino}-2-phenyl-1*H*-pyrazol-3(2*H*)-one

Chun-Hua Diao* and Xin Chen

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

Correspondence e-mail: diao_chunhua@163.com

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Key indicators

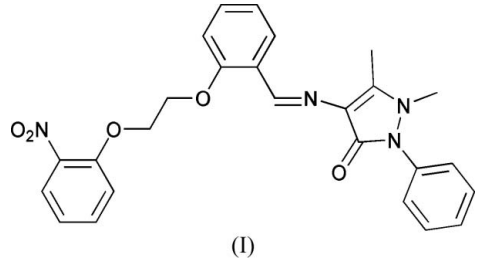
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.057
wR factor = 0.129
Data-to-parameter ratio = 13.1

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

In the title compound, $C_{26}H_{24}N_4O_5$, the salicylaldehyde group makes dihedral angles of 7.06 (10), 75.88 (9) and 37.62 (12)° with the pyrazolone ring, the terminal nitrobenzene ring and the terminal phenyl ring, respectively. The crystal packing is stabilized by π–π interactions and intermolecular C—H···O hydrogen bonds that form centrosymmetric dimers.

Comment

The synthesis and structure of Schiff bases have attracted attention in biology and chemistry (Kahwa *et al.*, 1986). Among the large number of compounds, 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of them, such as 4-[(2-hydroxy-3-methoxybenzyl-idene)amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Diao *et al.*, 2005) and (*E*)-4-[3-ethoxy-4-(2-phenoxyethoxy)-benzylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Zhang *et al.*, 2006), have been reported.



(I)

As part of an investigation of their crystal structures which will provide useful information for the coordination properties of Schiff bases functioning as ligands, we report here the synthesis and structure of the title compound, (I).

In the title molecule (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The pyrazolone ring (C16–C18/N2/N3/N4/O5) is almost planar, with an r.m.s. deviation for fitted atoms of 0.0314 Å. It makes a dihedral angle of 43.66 (10)° with the attached phenyl ring (C21–C26). The salicylaldehyde group (C9–C15/O4) is planar, with an r.m.s. deviation for fitted atoms of 0.0320 Å. This group makes dihedral angles of 7.06 (10), 75.88 (9) and 37.62 (12)°, respectively, with the the pyrazolone ring (C16–C18/N2/N3/N4/O5) and the terminal C1–C6 and C21–C26 nitrobenzene and phenyl rings.

The crystal packing is stabilized by weak non-classical intermolecular C—H···O hydrogen bonds (Table 1) that form centrosymmetric dimers (Fig. 2). In addition, π–π stacking interactions are observed between the C1–C6 nitrobenzene ring and the corresponding ring of the molecule at the

symmetry position $(1-x, -y, 2-z)$; the centroid–centroid distance between the two rings is 3.624 (1) Å.

Experimental

An anhydrous ethanol solution (30 ml) of 2-[2-(2-nitrophenoxy)ethoxy]benzaldehyde (2.87 g, 10 mmol) was added to an anhydrous ethanol solution (30 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a yellow precipitate. The product was then isolated, recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 85% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{26}H_{24}N_4O_5$
M_r = 472.49
Monoclinic, $P2_1/c$
a = 13.255 (4) Å
b = 18.369 (5) Å
c = 10.040 (3) Å
β = 103.140 (5)°
V = 2380.6 (12) Å^3
Z = 4
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, yellow
0.22 × 0.14 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.993
11202 measured reflections
4173 independent reflections
1986 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.129
S = 1.02
4173 reflections
318 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.3376P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O5^{i}	0.93	2.39	3.180 (4)	143

Symmetry code: (i) $-x+1, -y, -z+2$.

The H atoms were included in calculated positions and refined using a riding-model approximation. Constrained C—H bond lengths and isotropic U_{iso}(H) parameters: 0.93 Å and 1.2U_{eq}(C) for aromatic; 0.97 Å and 1.2U_{eq}(C) for methylene; 0.96 Å and 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*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

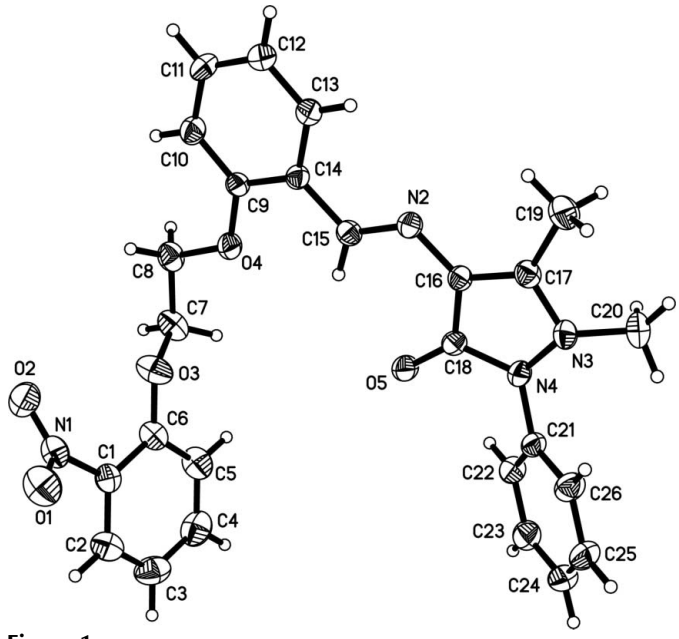


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

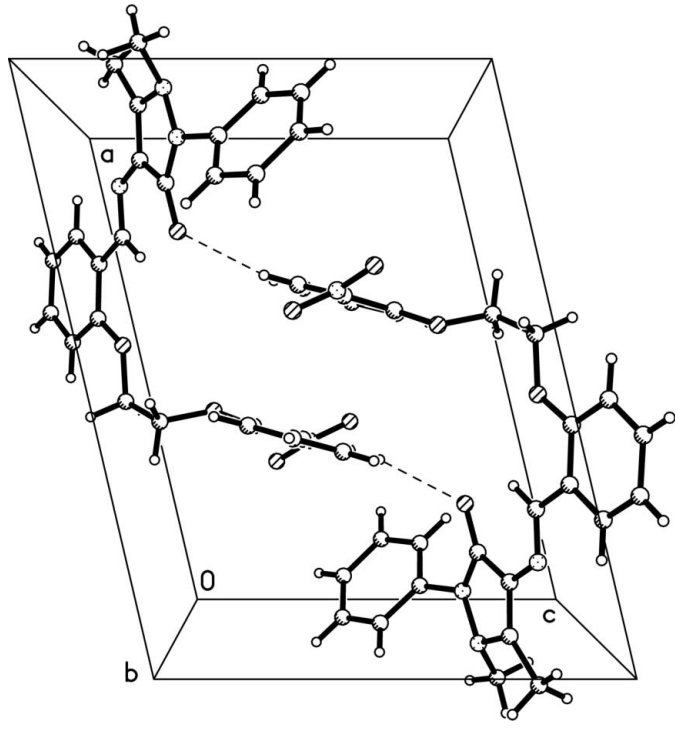


Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines) in (I).

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