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

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Key indicators

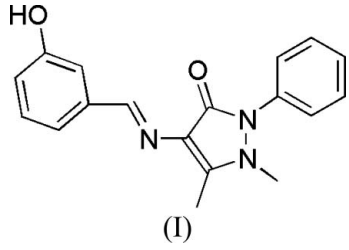
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.129
Data-to-parameter ratio = 17.2

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

The title compound, $C_{18}H_{17}N_3O_2$, was prepared using 3-hydroxybenzaldehyde and 4-amino-1,5-dimethyl-2-phenylpyrazolidin-3-one. The crystal structure of the title compound shows that intermolecular O—H···O hydrogen-bonding interactions link adjacent molecules and contribute to the stability of the structure in the solid state.

Comment

Metal complexes of Schiff bases have been studied extensively for purposes such as model compounds of active centres in various proteins and enzymes (Santos *et al.*, 2001). Investigation of their crystal structures may provide useful information concerning their physical and chemical properties. In the present study, we report the synthesis and structure of the title compound, (I).



(I)

In the molecular structure, the central system (N1–N3/C3–C6/C13/O1) is planar, with an r.m.s. deviation of fitted atoms of 0.0776 Å, and the dihedral angle with the phenyl ring (C7–C12) is 65.03 (7)°. The 3-hydroxybenzylidene group (C14–C20/O2) is planar, with an r.m.s. deviation of fitted atoms of 0.0157 Å; the dihedral angle with the central system is 7.51 (7)°. Intermolecular O—H···O hydrogen-bonding inter-

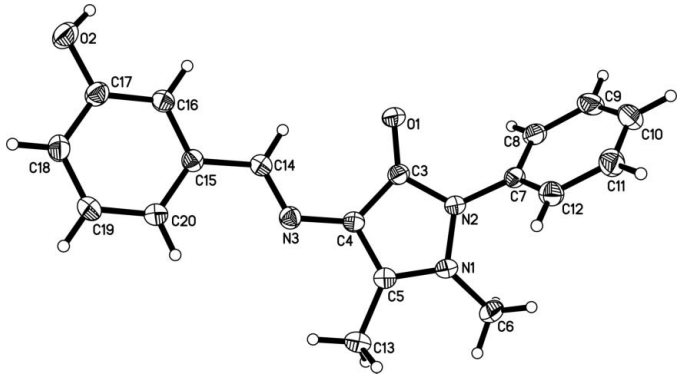


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

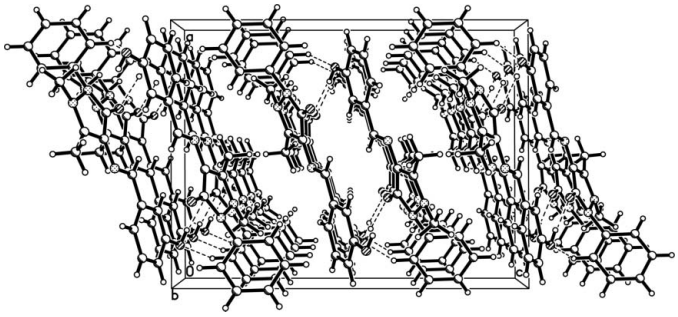


Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines).

actions are found, which play a key role in the stabilization of the crystal structure.

Experimental

An anhydrous ethanol solution of 3-hydroxybenzaldehyde (1.22 g, 10 mmol) was added to an anhydrous ethanol solution of 4-amino-1,5-dimethyl-2-phenylpyrazolidin-3-one (2.03 g, 10 mmol), and the mixture was stirred at 350 K for 5 h under nitrogen. A yellow precipitate appeared which was isolated, recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 92% yield. Bright-yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution of (I).

Crystal data

$C_{18}H_{17}N_3O_2$
M_r = 307.35
Monoclinic, $P2_1/c$
a = 12.885 (8) Å
b = 7.012 (4) Å
c = 17.109 (10) Å
β = 90.204 (8)°
V = 1545.8 (16) Å^3
Z = 4
D_x = 1.321 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3578 reflections
θ = 2.9–27.6°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, yellow
0.38 × 0.32 × 0.20 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.983
9740 measured reflections
3621 independent reflections
2743 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.8°
$h = -13 \rightarrow 16$
$k = -8 \rightarrow 9$
$l = -17 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.129
S = 1.05
3621 reflections
211 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.7122P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.91	2.727 (2)	175

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

The H atom attached to the O atom was located in a difference Fourier map and refined freely with an isotropic U parameter. Other H atoms were included in calculated positions and refined using a riding-model approximation. C—H bond lengths and isotropic U parameters were constrained: C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

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