Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Zuo-Liang Jing, Zhi Fan,* Ming Yu, Xin Chen and Qi-Liang Deng

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

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

Received 22 August 2005
Accepted 28 September 2005
Online 5 October 2005

The title compound, $C_{18}H_{19}N_3O_3$, was prepared using 4-hydroxybenzaldehyde and 4-amino-1,5-dimethyl-2-phenylpyrazolidin-3-one. The crystal structure shows that the title compound includes a water molecule, which forms O—H···O hydrogen bonds with adjacent molecules and plays an important role in the stabilization of the crystal structure.

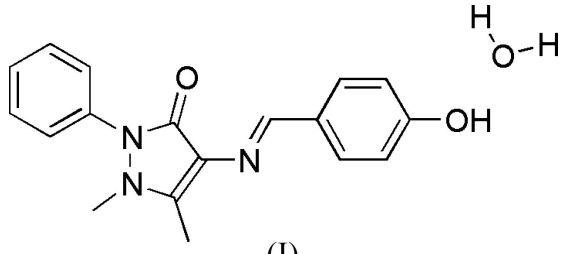
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.103
Data-to-parameter ratio = 12.4

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

Comment

In order to investigate their potential pharmacological activity (Parashar *et al.*, 1988) and photochromic properties (Hadjoudis *et al.*, 1987), a large number of metal complexes of Schiff bases have been synthesized. As part of these studies, we report the synthesis and molecular structure of the title compound, (I).



(I)

In the molecular structure, the central system (N1–N3/C3–C6/C13/O2) is planar, with an r.m.s. deviation of fitted atoms of 0.0451 Å, and the dihedral angle with the phenyl ring (C7–C12) is 89.93 (4)°. The phenol group (C15–C20/O1) is planar, with an r.m.s. deviation of fitted atoms of 0.0108 Å, and the dihedral angle with the central system is 4.82 (6)°. These values are in agreement with those in a similar system (Diao *et al.*, 2005). It is noted that the water molecules interact with pyrazolone molecules through hydrogen bonds (Table 1), which contribute to the stability of the structure in the solid state (Fig. 2).

Experimental

An anhydrous ethanol solution of 4-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 83% yield. Bright-yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution of (I).

Crystal data

$C_{18}H_{17}N_3O_2\cdot H_2O$	$Z = 2$
$M_r = 325.36$	$D_x = 1.327$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.393$ (2) Å	Cell parameters from 2426 reflections
$b = 8.983$ (3) Å	$\theta = 2.6$–$27.7°$
$c = 12.823$ (4) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 77.510$ (4)°	$T = 294$ (2) K
$\beta = 82.756$ (3)°	Block, yellow
$\gamma = 79.450$ (3)°	0.52 × 0.46 × 0.34 mm
$V = 814.1$ (4) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	2843 independent reflections
φ and ω scans	2407 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	$R_{int} = 0.014$
$T_{min} = 0.923$, $T_{max} = 0.969$	$\theta_{max} = 25.0°$
4423 measured reflections	$h = -8 \rightarrow 8$
	$k = -9 \rightarrow 10$
	$l = -15 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.1768P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.103$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
2843 reflections	Extinction correction: *SHELXL97*
229 parameters	Extinction coefficient: 0.082 (6)
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3	0.94 (2)	1.69 (2)	2.6348 (18)	178 (2)
O3—H3A···O1^{i}	0.83 (3)	2.27 (3)	3.0182 (19)	149 (3)
O3—H3B···O2^{ii}	0.91 (3)	1.81 (3)	2.7076 (18)	168 (3)

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

The H atoms of the hydroxyl group and water molecule were found in a difference Fourier map and refined freely with an isotropic U parameter. Other H atoms were included in calculated positions and refined as riding. 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, 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*.

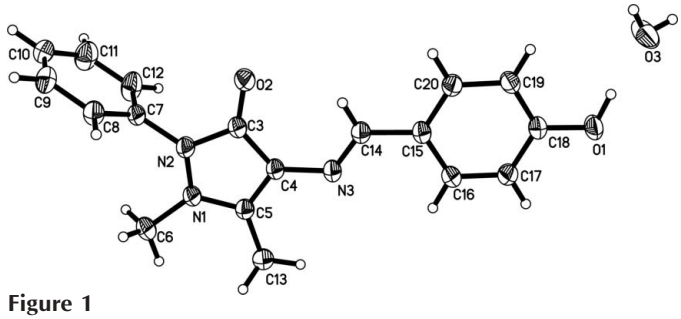


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

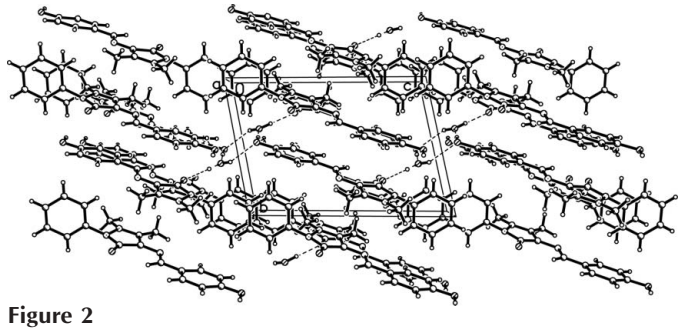


Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines).

This work was supported by the Science Fund of Tianjin University of Science and Technology (grant No. 118181), which is gratefully acknowledged.

References

Bruker (1999). *SADABS*, *SMART* and *SAINT*. 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.
Hadjoudis, E., Vittorakis, M. & Moustakali-Mavridis, J. (1987). *Tetrahedron*, **43**, 1345–1360.
Parashar, R. K., Sharma, R. C., Kumar, A. & Mohan, G. (1988). *Inorg. Chim. Acta*, **151**, 201–208.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.