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(*E*)-4-(5-Bromo-2-hydroxybenzylideneamino)-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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In the crystal structure of the title Schiff base compound, $C_{18}H_{16}BrN_3O_2$, there are three hydrogen bonds which stabilize the molecular and crystal structures.

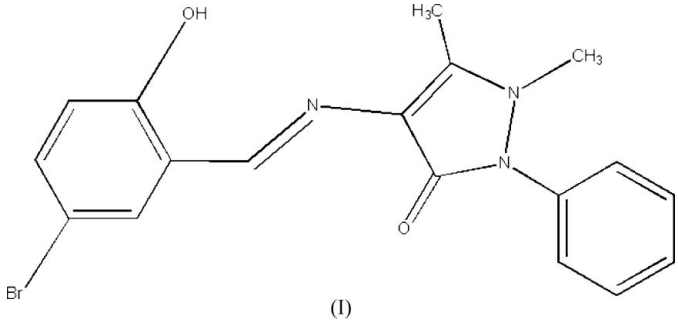
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.095
Data-to-parameter ratio = 14.9

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

Comment

Schiff bases showing solvent-dependent UV–vis spectra (solvatochromicity) can be suitable non-linear optical (NLO) active materials (Alemi & Shaabani, 2000). They are also useful in the asymmetric oxidation of methylphenylsulfide and are enantioselective (Kim & Shin, 1999). We report here the synthesis and crystal structure of the title compound (I) (Fig. 1). The crystal structures of similar Schiff bases and of a Cu complex based on such a Schiff base have been reported previously by us (Yan, Yang *et al.*, 2006; Yan, Zheng *et al.*, 2006; Yang, Yan *et al.*, 2006; Yang, Zhang *et al.*, 2007; Zheng *et al.*, 2006).



(I)

In the crystal structure of (I), there are two intramolecular hydrogen bonds (Table 1) which stabilize the molecular structure, while one intermolecular hydrogen bond stabilizes the crystal structure, forming a chain running along the *b* axis (Fig. 2).

Experimental

A mixture of 4-amino-1,5-dimethyl-2-phenyl-1,2-dihydropyrazol-3-one (2.08 g, 10 mmol), Na_2SO_4 (3.0 g) and 5-bromosalicylaldehyde (1.32 g, 10 mmol) in absolute ethanol (20 ml) was refluxed under nitrogen for about 12 h, yielding a yellow precipitate. The product was filtered off and washed with ethanol. The crude solid was dissolved in CH_2Cl_2 (100 ml), washed with water (2 × 10 ml) and brine (10 ml), and dried over Na_2SO_4. The remaining solvent was removed under vacuum (yield 92%, 3.1 g). Colourless single crystals of (I) suitable for X-ray analysis were grown by slow evaporation of a CH_2Cl_2–absolute ethanol (4:1 *v*/*v*) solution at room temperature over a period of about a week.

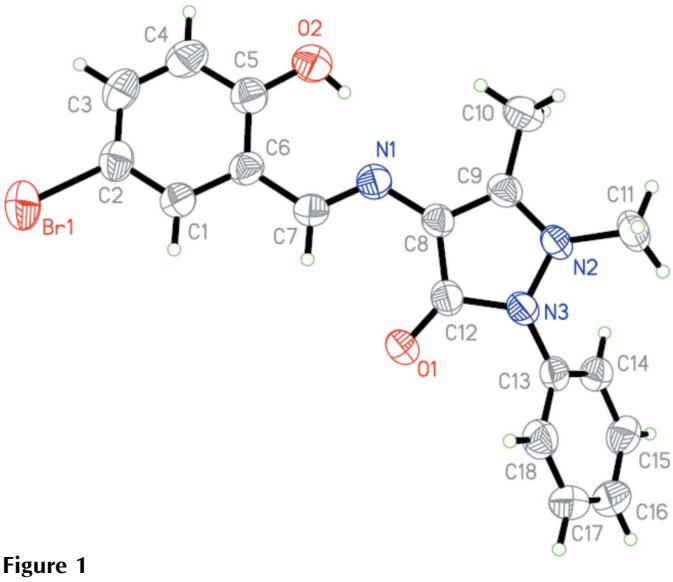


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 50% probability displacement ellipsoids.

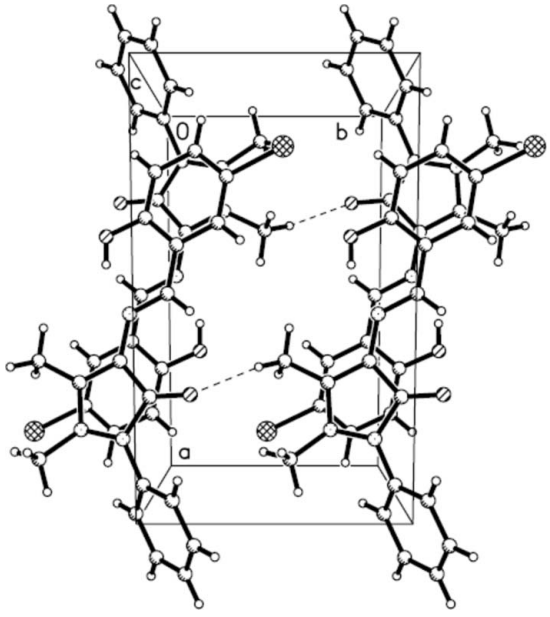


Figure 2
A packing diagram for (I), viewed down the *c* axis. C—H···O hydrogen bonds are indicated by dashed lines.

Crystal data

$C_{18}H_{16}BrN_3O_2$
M_r = 386.25
Monoclinic, $P2_1/n$
a = 12.1187 (5) Å
b = 7.0788 (3) Å
c = 20.3250 (9) Å
β = 104.458 (1)°
V = 1688.38 (12) Å^3
Z = 4
D_x = 1.520 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.45 mm^{-1}
T = 293 (2) K
Block, colourless
0.46 × 0.37 × 0.34 mm

Data collection

Bruker APEXII area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.358, T_{max} = 0.435
10580 measured reflections
3273 independent reflections
2248 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 0.94
3273 reflections
220 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O1^{i}	0.96	2.45	3.398 (3)	171
C7—H7···O1	0.93	2.37	3.039 (3)	128
O2—H2···N1	0.82	1.87	2.596 (3)	146

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

All H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å and O—H = 0.82 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C and O).

Data collection: *SMART* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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References

Alemi, A. A. & Shaabani, B. (2000). *Acta Chim. Slov.* **47**, 363–369.
Bruker (1998). *SMART* (Version 5.0) and *SHELXTL* (Version 5.10). Bruker AXS Inc, Madison, Wisconsin, USA.
Bruker (1999). *SAINT* (Version 6.12). Bruker AXS Inc., Madison, Wisconsis, USA.
Kim, G. J. & Shin, J. W. (1999). *Catal. Lett.* **63**, 83–89.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yan, G.-B., Yang, M.-H. & Zheng, Y.-F. (2006). *Acta Cryst.* E**62**, m3481–m3482.
Yan, G.-B., Zheng, Y.-F., Zhang, C.-N. & Yang, M.-H. (2006). *Acta Cryst.* E**62**, o5328–o5329.
Yang, M.-H., Yan, G.-B., Zheng, Y.-F. & Zhang, C.-N. (2006). *Acta Cryst.* E**62**, o4944–o4945.
Yang, M.-H., Zhang, C.-N., Yan, G.-B., Zheng, Y.-F. & Liu, X.-B. (2007). *Acta Cryst.* E**63**, o382–o383.
Zheng, Y.-F., Yan, G.-B. & Gu, Y.-B. (2006). *Acta Cryst.* E**62**, o5134–o5135.