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4-[(2-Hydroxyphenylamino)phenylmethylene]-5-methyl-2-phenyl-2*H*-pyrazol-3(4*H*)-one

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Key indicators

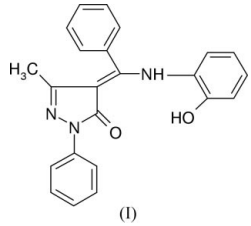
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.141
Data-to-parameter ratio = 11.1

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

The title compound, $C_{23}H_{19}N_3O_2$, a condensation product of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone and *o*-aminophenol, is a neutral tridentate ligand in enamine–keto form, due to a strong intramolecular N—H···O hydrogen bond. A pair of intermolecular O—H···O hydrogen bonds link molecules to give dimers.

Comment

A view of the molecular structure of the title compound, (I), is shown in Fig. 1. The compound was prepared from the reaction of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone (PMBP) and *o*-aminophenol, forming this tridentate ligand. In the pyrazole ring, the bond lengths C1—C2, C2—C3, C3—N1, N1—N2 and N2—C1 (Table 1) lie between classical single- and double-bond lengths. The bond angles within this ring deviate by up to 4° from the 108° angle of a regular pentagon.



(I)

The bond lengths O1—C1, C2—C5, C1—C2 and C5—N3 also lie between classical single- and double-bond lengths. Atoms O1, C1, C2, C5 and N3 are essentially coplanar, the largest deviation from the mean plane being 0.020 (2) Å for C5. The dihedral angle between this mean plane and that of the pyrazoline ring is 5.05 (3)°, indicating a high degree of conjugation and electron delocalization. The dihedral angles between the first mean plane and phenyl rings C11—C16, C21—C26 and C31—C36 are 45.91 (3), 113.79 (4) and 129.96 (4)°, respectively, because of steric hindrance effects. The C11—N2—N1—C3 torsion angle is −4.7 (3)°, different from the value of 16.7 (3)° in 3-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenylpyrazol-4-ylmino)-4,4,4-trifluoro-1-(2-thienyl)-butane-1,2-dione (Wang *et al.*, 2002). Small torsion angles for C1—C2—C5—N3 [−2.6 (4)°] and N3—C31—C32—O2 [−4.8 (4)°] show that atoms O1, N3 and O2 are in a *cis* conformation and can act as the coordinating atoms of a tridentate ligand.

A strong intramolecular N3—H3···O1 hydrogen bond is found (Table 2), resulting in an enamine–keto tautomeric form. Pairs of intermolecular O—H···O hydrogen bonds link molecules into centrosymmetric dimers, with the formation of a 14-membered ring (Fig. 2).

Experimental

Ethanol solutions of 0.1 mol of PMBP and 0.1 mol of *o*-aminophenol were refluxed together for 4 h over a steam bath. The excess solvent was removed by evaporation and the concentrated solution was cooled in an ice bath with stirring. The title compound separated out as a cream powder, which was collected and dried in air. Bright-yellow single crystals, suitable for X-ray analysis, were obtained by slow cooling of a warmed ethanol solution, and were dried in a vacuum over $CaCl_2$. The product is stable in air, and soluble in acetone and ethanol. Elemental analysis: calculated C 74.78, H 5.19, N 11.41%; found C 74.63, H 5.09, N 11.41%.

Crystal data

$C_{23}H_{19}N_3O_2$	$Z = 2$
$M_r = 369.41$	$D_x = 1.243$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.267$ (4) Å	Cell parameters from 2764 reflections
$b = 11.150$ (6) Å	$\theta = 1.7$–$25.1°$
$c = 13.822$ (8) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 111.794$ (9)°	$T = 293$ (2) K
$\beta = 92.210$ (11)°	Prism, yellow
$\gamma = 105.987$ (10)°	0.30 × 0.25 × 0.20 mm
$V = 987.2$ (10) Å^3	

Data collection

Bruker SMART 1000 CCD diffractometer	1687 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.024$
ω scans	$\theta_{max} = 23.3°$
Absorption correction: none	$h = -8 \rightarrow 8$
3405 measured reflections	$k = -12 \rightarrow 12$
2830 independent reflections	$l = -9 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.0157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.051$	
$wR(F^2) = 0.141$	
$S = 0.98$	$(\Delta/\sigma)_{max} = 0.005$
2830 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
254 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.012 (3)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.278 (3)	N3—C5	1.340 (4)
N1—C3	1.326 (4)	C1—C2	1.444 (4)
N1—N2	1.423 (3)	C2—C5	1.411 (4)
N2—C1	1.379 (3)	C2—C3	1.449 (4)
C3—N1—N2	105.6 (2)	C1—C2—C3	105.0 (2)
C1—N2—N1	111.9 (2)	N1—C3—C2	111.8 (3)
N2—C1—C2	105.5 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1	0.86	2.01	2.750 (3)	143
O2—H2···O1^{i}	0.82	1.96	2.724 (3)	155

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

H atoms were placed geometrically and refined with riding-model constraints.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

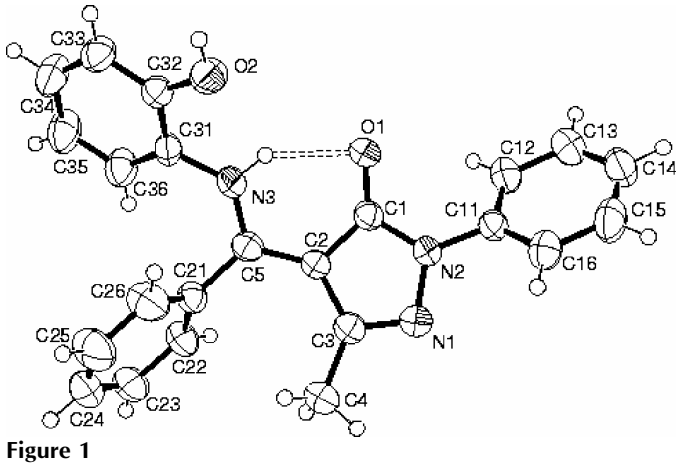


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids. The intramolecular hydrogen bond is represented by dashed lines.

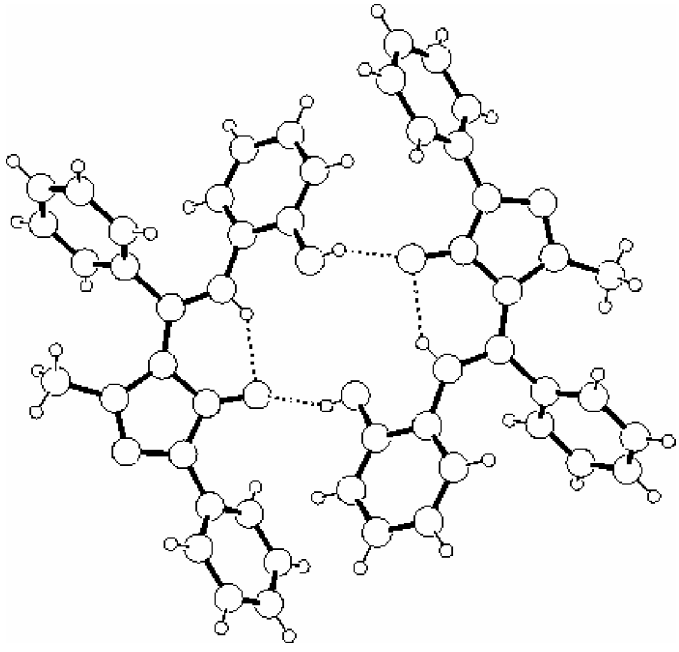


Figure 2
A centrosymmetric dimer formed by hydrogen bonds (shown dashed).

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