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3-Phenyl-1-(2-pyridyl)-1*H*-pyrazol-5-ol

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.136
Data-to-parameter ratio = 29.6

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

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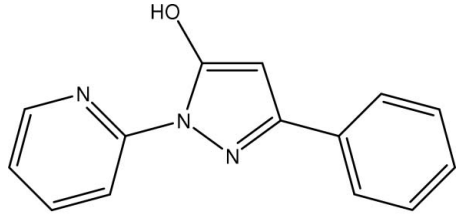
In the title compound, $C_{14}H_{11}N_3O$, there is an intramolecular O—H···N hydrogen bond enforcing coplanarity of the pyrazole and pyridine rings, with O—H = 1.013 (18) Å, H···N = 1.659 (18) Å, O···N = 2.5767 (14) Å, and O—H···N = 148.3 (15)°.

Comment

In non-polar solvents, pyrazoles of this type tend to be in the keto form, but when crystallized from polar solvents (as in the present case), they display the enol form. The title compound, (I), consists of a pyrazole ring substituted at the 1-, 3- and 5-positions by a 2-pyridyl ring, a phenyl ring and a hydroxyl group, respectively.



(I)

The pyridine ring is nearly coplanar with the pyrazole ring [2.69 (9)°]. Coplanarity is enforced, in part, by an intramolecular O—H···N hydrogen bond (Table 2), although the same pyridine–pyrazole dihedral angle (2.60°) is found in a similar but non-hydrogen-bonded system (Bessel *et al.*, 1992). The phenyl ring plane is twisted by 27.10 (7)° with respect to the pyrazole ring plane.

Experimental

Following a general procedure first reported by Knorr (1887), 2-pyridylhydrazine (2 g, 18.3 mmol) was added to a solution of ethyl benzoylacetate (3.5 g, 18.3 mmol) in acetic acid (20 ml) and refluxed for 18 h. After cooling, no crystallization occurred so water and ethanol (20 ml each) were added and the solution was allowed to stand. Yellow crystals of the title compound formed (yield 3.2 g, 74%; m.p. 383–386 K).

Crystal data

$C_{14}H_{11}N_3O$
M_r = 237.26
Monoclinic, $P2_1/c$
a = 9.618 (2) Å
b = 10.538 (2) Å
c = 11.482 (3) Å
β = 104.215 (10)°
V = 1128.1 (4) Å^3
Z = 4
D_x = 1.397 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 K
Parallelepiped, yellow
0.40 × 0.33 × 0.25 mm

Data collection

Nonius KappaCCD diffractometer with an Oxford Cryosystems Cryostream cooler
ω scans with κ offsets
Absorption correction: none
9591 measured reflections
4948 independent reflections
2653 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 35.1^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.136$
$S = 0.98$
4948 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.3406 (13)	C3—N2	1.3330 (15)
C1—C2	1.3614 (17)	C3—C4	1.4769 (16)
C1—N1	1.3855 (14)	C10—N1	1.3994 (15)
C2—C3	1.4182 (16)	N1—N2	1.3787 (13)
O1—C1—C2	130.96 (11)	C2—C3—C4	127.45 (10)
O1—C1—N1	121.64 (10)	N2—N1—C1	111.15 (9)
C2—C1—N1	107.40 (10)	N2—N1—C10	121.40 (9)
C1—C2—C3	104.76 (10)	C1—N1—C10	127.35 (9)
N2—C3—C2	112.65 (10)	C3—N2—N1	104.03 (9)
N2—C3—C4	119.88 (10)	C1—O1—H1*O*	104.5 (10)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N3	1.013 (18)	1.659 (18)	2.5767 (14)	148.3 (15)

The H(O) atom was refined independently. All H(C) atoms were placed in calculated positions, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C), and thereafter treated as riding.

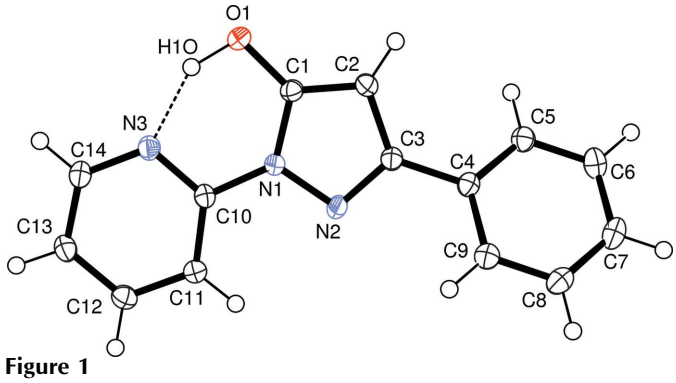


Figure 1
View of (I), shown with 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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