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4-(5-Methyl-1*H*-pyrazol-3-yl)pyridine monohydrate

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In the title molecule, $C_9H_9N_3\cdot H_2O$, the dihedral angle between the planes of the pyridine and pyrazole rings is 27.52 (2)°. In the crystal structure, intermolecular N—H···O, O—H···N and weak C—H···O hydrogen bonds help stabilize the crystal structure.

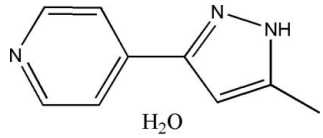
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.133
Data-to-parameter ratio = 14.4

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

Comment

4-(5-Methyl-1*H*-pyrazol-3-yl)pyridine and its derivatives are the subject of intensive study as ligands with N and S donor sets (Ibrahim *et al.*, 2006). In the present paper, we report the crystal structure of 4-(5-methyl-1*H*-pyrazol-3-yl)pyridine, which crystallizes as a monohydrate, (I) (Fig. 1). The bond lengths and angles are within the normal ranges (Allen *et al.*, 1987). The dihedral angle between the planes of the pyridine and pyrazole rings is 27.52 (2)°. Intermolecular N—H···O, O—H···N and C—H···O hydrogen bonds help stabilize the crystal structure (Table 1, Fig. 2).



(I)

Experimental

The title compound, (I), was prepared according to the method of Tarrago *et al.* (1980). A 250 ml round-bottomed flask was charged with 16.32 g (0.1 mol) of 4-acetoacetylpyridine and 100 ml of absolute ethanol. Into the stirred mixture, aqueous hydrazine hydrate (6.25 g, 0.1 mol, 80%) was added dropwise. This mixture was stirred at room temperature for another 3 h and filtered. The resulting crystals were recrystallized from absolute ethanol and then from a mixture of ethanol and petroleum ether (1:1 *v*/*v*).

Crystal data

$C_9H_9N_3\cdot H_2O$
M_r = 177.21
Monoclinic, $P2_1/c$
a = 7.568 (2) Å
b = 8.621 (3) Å
c = 14.704 (4) Å
β = 95.652 (5)°
V = 954.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
0.28 × 0.14 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.990
4391 measured reflections
1756 independent reflections
1174 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

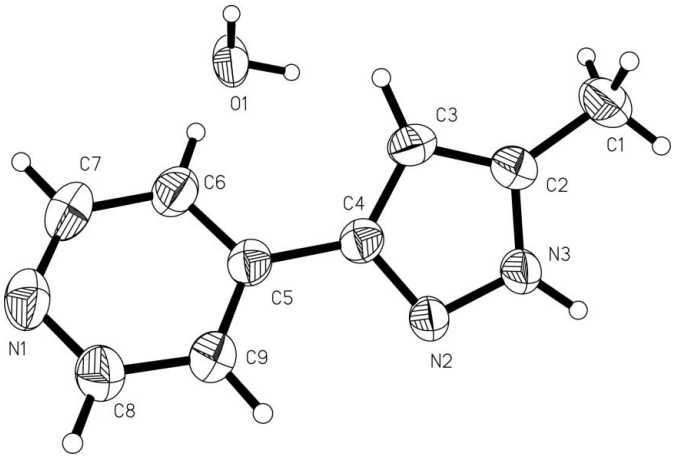


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 40% probability level.

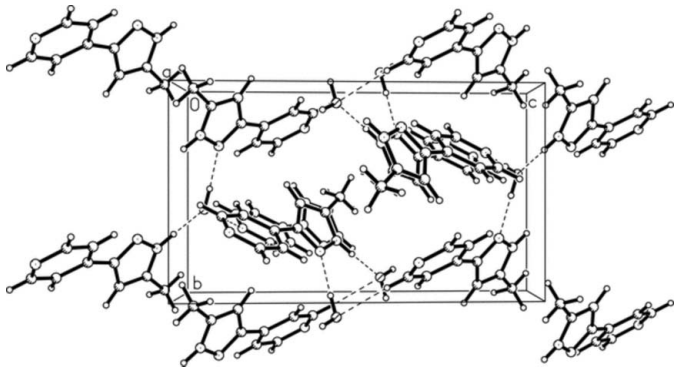


Figure 2
Partial packing plot of (I). Hydrogen bonds are shown as dashed lines.

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.133$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 0.99$	$\Delta\rho_{min} = -0.16$ e Å^{-3}
1756 reflections	
122 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.95	2.55	3.450 (3)	159
O1—H2···N2^{ii}	0.91	1.94	2.844 (3)	170
N3—H3A···O1^{iii}	0.95	1.77	2.724 (2)	178

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

All C-bound H atoms were placed in calculated positions, with C—H = 0.95 or 0.98 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) values of $1.2U_{eq}$(C) for aromatic H atoms and $1.5U_{eq}$(C) for methyl H atoms. N-bound and O-bound H atoms were refined as riding in their as-found positions with the U_{iso}(H) values refined freely (N—H = 0.95 Å, and O—H = 0.91 and 0.94 Å).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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