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1-(Hydroxymethyl)-3,5-dimethylpyrazole

Ivana Radosavljević Evans,[a]* Katalin Mészáros Szécsényi[b] and Vukadin M. Leovac[b]

[a]Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, England, and [b]Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovica 3, 21000 Novi Sad, Serbia and Montenegro

Correspondence e-mail:
ivana.radosavljevic@durham.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.001 Å
R factor = 0.040
wR factor = 0.100
Data-to-parameter ratio = 17.3

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

The structure of the title compound, $C_6H_{10}N_2O$, has been determined from single crystals obtained by recrystallization from acetone. Intermolecular O—H···N hydrogen bonding gives rise to $R_2^2(10)$ dimers.

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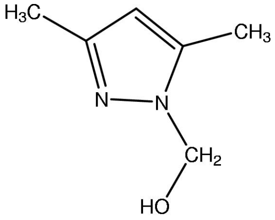
Comment

1-(Hydroxymethyl)-3,5-dimethylpyrazole (H*L*), (I), was first synthesized by a reaction of 3,5-dimethylpyrazole with paraformaldehyde (Driessen, 1982). H*L* can act as a chelating ligand, as shown by the examples of four isomorphous cubane-type cluster coordination compounds of the formula $[MXL(\text{EtOH})_4]$ (M = Co^{II}, Ni^{II}, X = Cl, Br; Paap *et al.*, 1985), where the deprotonated species acts as a bidentate ligand, coordinating the metals through its pyridine N atom and the methoxy O atom. With a metal with different coordination preferences, such as Pd, H*L* acts as a monodentate ligand through the pyrazole N atom, forming a square-planar complex (Boixassa *et al.*, 2002).



(I)

The molecular structure of (I) is shown in Fig. 1. The substituted pyrazole ring is essentially planar, the largest displacement being 0.01 Å for C4. The O1—C1—N1—N2 torsion angle is 90.19 (9)°. The structure is stabilized by intermolecular O—H···N hydrogen bonding between adjacent molecules [H···N = 1.89 (2) Å, O···N = 2.760 (1) Å and O—H···N = 171.0 (2)°]. These interactions give rise to dimers

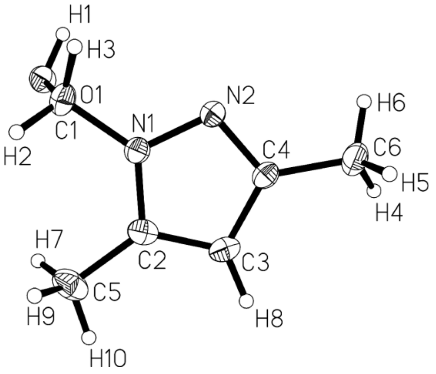


Figure 1
The molecular structure of (I) and the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

with an $R_2^2(10)$ hydrogen-bonding motif (Etter *et al.*, 1990) (Fig. 2).

Experimental

Needle-shaped clear single crystals of (I) were obtained by recrystallization of the commercial product (Aldrich) from acetone.

Crystal data

$C_6H_{10}N_2O$
$M_r = 126.16$
Monoclinic, $P2_1/n$
$a = 7.2877$ (2) Å
$b = 11.9265$ (3) Å
$c = 8.1586$ (2) Å
$\beta = 107.396$ (1)°
$V = 676.68$ (3) Å^3
$Z = 4$
$D_x = 1.238$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6570 reflections
$\theta = 3.1$–$34.3°$
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Needle, white
0.80 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.92$, $T_{\max} = 0.98$
13356 measured reflections
2742 independent reflections
2113 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 34.5°$
$h = -11 \rightarrow 11$
$k = -18 \rightarrow 19$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.100$
$S = 1.00$
2113 reflections
122 parameters
All H-atom parameters refined
$w = [1 - (F_o - F_c)/6\sigma(F_o)^2]^2/[3.44T_0(x) + 4.59T_1(x) + 1.31T_2(x)]$ where T are the Chebychev polynomial terms and $x = F_c/F_{\max}$ (Watkin, 1994; Prince, 1982)
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.40$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.4007 (10)	C2—C5	1.4918 (13)
N1—C1	1.4530 (11)	C3—C2	1.3814 (13)
N1—C2	1.3568 (11)	C3—C4	1.4073 (12)
N2—N1	1.3627 (10)	C6—C4	1.4934 (12)
N2—C4	1.3362 (10)		
N1—N2—C4	105.40 (7)	C3—C2—N1	106.36 (7)
N2—N1—C1	119.71 (7)	C3—C2—C5	131.14 (8)
N2—N1—C2	111.90 (7)	N1—C2—C5	122.49 (8)
C1—N1—C2	128.31 (7)	C6—C4—C3	128.72 (8)
N1—C1—O1	112.93 (7)	C6—C4—N2	120.72 (8)
C2—C3—C4	105.78 (7)	C3—C4—N2	110.55 (7)

H atoms were found in a difference Fourier map and refined using an isotropic approximation. Refined C—H bond lengths are in the range 0.95 (2)–1.04 (2) Å and the O—H bond length is 0.88 (2) Å.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ATOMS* (Dowty, 2000); software used to prepare material for publication: *CRYSTALS*.

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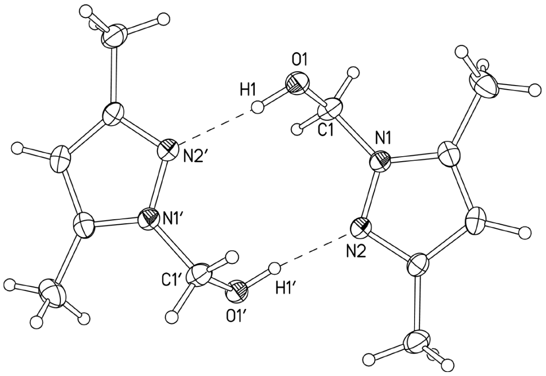

Figure 2
The hydrogen bonding (dashed lines) in (I).

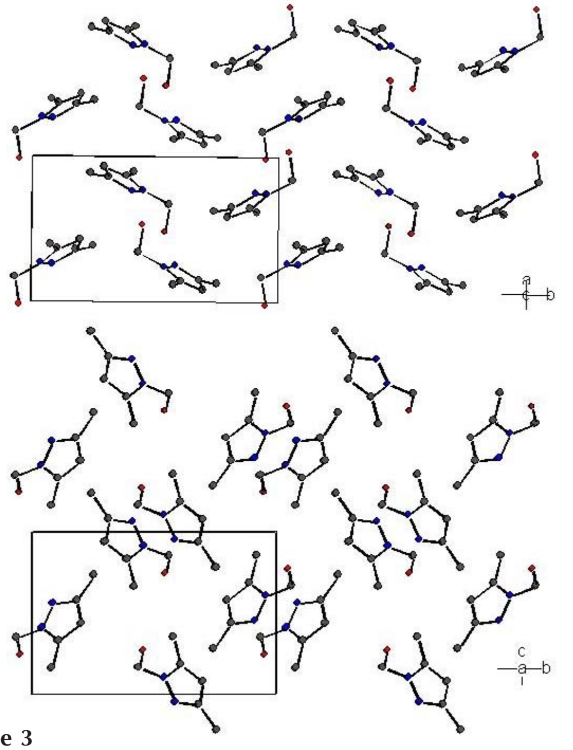

Figure 3
Two views of the packing scheme in (I).

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