Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

4-Hydroxymethyl-3,5-dimethyl-1*H*-pyrazole

Guo-Bing Yan

Department of Chemistry, Lishui College, 323000 Lishui, ZheJiang, People's Republic of China
Correspondence e-mail: jgschl@126.com

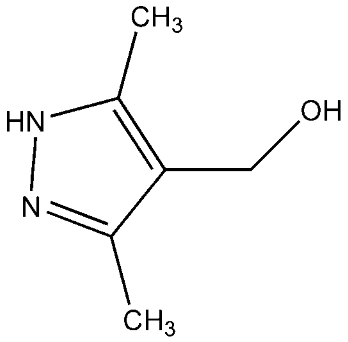
Received 27 April 2007; accepted 3 May 2007

Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.048; *wR* factor = 0.148; data-to-parameter ratio = 15.1.

In the title compound, $C_6H_{10}N_2O$, corrugated sheets parallel to the (101) plane are formed *via* intermolecular O—H···N and N—H···O hydrogen-bonding interactions.

Related literature

For related literature, see: Kozlevcar *et al.* (2006); Moncol *et al.* (2006).



Experimental

Crystal data

$C_6H_{10}N_2O$
$M_r = 126.16$
Monoclinic, $P2_1/n$
$a = 8.2608\ (12)$ Å
$b = 8.3865\ (12)$ Å
$c = 9.9672\ (14)$ Å
$\beta = 91.311\ (2)^\circ$
$V = 690.34\ (17)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 298\ (2)$ K
0.38 × 0.30 × 0.22 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.955$, $T_{max} = 0.977$
5091 measured reflections
1284 independent reflections
1106 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.148$
$S = 1.06$
1284 reflections
85 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.98	2.7965 (18)	177
N2—H2···O1^{ii}	0.86	1.98	2.842 (2)	179

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 2004); software used to prepare material for publication: *SHELXTL*.

The author gratefully acknowledges financial support from the Youth Foundation of Lishui College (grant No. QN05004).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2170).

References

Bruker (2004). *APEX2* (Version 6.12), *SAINT* (Version 6.10) and *SHELXTL* (Version 5.0). Bruker AXS Inc, Madison, Wisconsin, USA.
Kozlevcar, B., Odlazek, D., Golobic, A., Pevec, A., Strauch, P. & Segedin, P. (2006). *Polyhedron*, **25**, 1161–1166.
Moncol, J., Púčeková, Z., Lis, T. & Valigura, D. (2006). *Acta Cryst.* E**62**, m448–m450.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

doi:10.1107/S1600536807021836

supplementary materials

Acta Cryst. (2007). E**63**, o2889 [**doi:10.1107/S1600536807021836**]

4-Hydroxymethyl-3,5-dimethyl-1*H*-pyrazole

G.-B. Yan

Comment

Hydrogen-bonding interactions between ligands are specific and directional and are, when present in metal complexes, usually not dependent on the properties of the metal ions, but they are playing a critical role in the structures and functions of the complexes. In this sense, 4-hydroxymethyl-3,5-dimethylpyrazole is an excellent candidate for the construction of supramolecular complexes, since it not only has multiple coordination modes but also can form regular hydrogen bonding by functioning as both a hydrogen-bonding donor and acceptor. (Moncol *et al.*, 2006; Kozlevcar *et al.*, 2006).

The molecular structure of (I) is depicted in Fig. 1. The C—O, C—C and C—N distances show no remarkable features, with C—N distances in the range of 1.336 (2)–1.343 (2) Å. The intermolecular O—H···N and N—H···O hydrogen bonds (Table 1) lead to the formation of a zig-zag like layer structure developping parallel to the (1 0 1) plane.

Experimental

4-hydroxymethyl-3,5-dimethylpyrazole was dissolved in hot methanol with stirring. The colourless single crystals suitable for X-ray diffraction were obtained at room temperature by slow evaporation of the solvent over several days.

Refinement

All H atoms were placed in calculated positions (C—H = 0.96 or 0.97 /%A; O—H = 0.82 /%A; N—H = 0.86 /%A) refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C, N) for aromatic ring and methylene, U_{iso}(H) = 1.5U_{eq}(C, O) for methyl and hydroxyl groups.

Figures

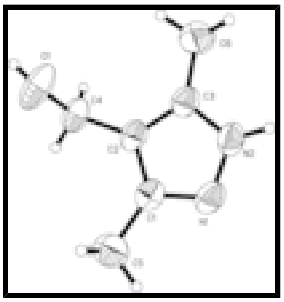


Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacements ellipsoids are drawn at the 50% probability level. H atoms are depicted as spheres of arbitrary radii.

4-Hydroxymethyl-3,5-dimethyl-1*H*-pyrazole

Crystal data

$C_6H_{10}N_2O$	F_{000} = 272

$M_r = 126.16$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.2608\ (12)$ Å

$b = 8.3865\ (12)$ Å

$c = 9.9672\ (14)$ Å

$\beta = 91.311\ (2)^\circ$

$V = 690.34\ (17)$ Å^3

$Z = 4$

$D_x = 1.214$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 2400 reflections

$\theta = 1.4–26.0^\circ$

$\mu = 0.09$ mm^{-1}

$T = 298\ (2)$ K

Block, colourless

0.38 × 0.30 × 0.22 mm

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2)$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.955$, $T_{\max} = 0.977$

5091 measured reflections

1284 independent reflections

1106 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

$\theta_{\max} = 25.5^\circ$

$\theta_{\min} = 3.2^\circ$

$h = -9 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.148$

$S = 1.06$

1284 reflections

85 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0866P)^2 + 0.1946P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.30$ e Å^{-3}

$\Delta\rho_{\min} = -0.27$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	1.01921 (18)	0.08862 (18)	0.73825 (14)	0.0474 (4)
N2	0.86594 (19)	0.03797 (18)	0.71167 (14)	0.0482 (4)
H2	0.8369	−0.0125	0.6400	0.058*
C1	1.0139 (2)	0.16032 (19)	0.85775 (16)	0.0429 (4)
C2	0.8560 (2)	0.15464 (18)	0.90737 (16)	0.0410 (4)
C3	0.7647 (2)	0.0757 (2)	0.81028 (16)	0.0443 (4)
C4	0.7974 (2)	0.2163 (2)	1.03853 (17)	0.0497 (5)
H4A	0.7174	0.1434	1.0733	0.060*
H4B	0.8874	0.2212	1.1026	0.060*
C5	1.1609 (2)	0.2342 (3)	0.9195 (2)	0.0621 (6)
H5A	1.2546	0.2009	0.8716	0.093*
H5B	1.1717	0.2013	1.0115	0.093*
H5C	1.1516	0.3482	0.9153	0.093*
C6	0.5902 (3)	0.0310 (3)	0.8047 (2)	0.0667 (6)
H6A	0.5510	0.0342	0.7133	0.100*
H6B	0.5296	0.1048	0.8575	0.100*
H6C	0.5774	−0.0748	0.8398	0.100*
O1	0.7283 (2)	0.36867 (16)	1.02448 (13)	0.0678 (5)
H1	0.6660	0.3845	1.0860	0.102*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0503 (9)	0.0473 (8)	0.0452 (8)	−0.0004 (6)	0.0171 (6)	−0.0007 (6)
N2	0.0558 (9)	0.0515 (9)	0.0377 (8)	−0.0043 (7)	0.0111 (6)	−0.0073 (6)
C1	0.0497 (10)	0.0374 (8)	0.0419 (9)	0.0019 (7)	0.0087 (7)	0.0030 (7)
C2	0.0502 (10)	0.0376 (8)	0.0355 (8)	0.0016 (7)	0.0104 (7)	0.0013 (6)
C3	0.0476 (10)	0.0462 (9)	0.0395 (9)	−0.0011 (7)	0.0110 (7)	0.0007 (7)
C4	0.0655 (12)	0.0472 (10)	0.0369 (9)	0.0071 (8)	0.0131 (8)	0.0008 (7)
C5	0.0555 (12)	0.0620 (12)	0.0688 (13)	−0.0054 (9)	−0.0010 (9)	−0.0006 (10)
C6	0.0517 (12)	0.0837 (15)	0.0652 (13)	−0.0084 (10)	0.0092 (9)	−0.0069 (11)
O1	0.1014 (12)	0.0557 (9)	0.0479 (8)	0.0278 (7)	0.0356 (7)	0.0115 (6)

Geometric parameters (Å, °)

N1—C1	1.336 (2)	C4—H4A	0.9700
N1—N2	1.356 (2)	C4—H4B	0.9700
N2—C3	1.343 (2)	C5—H5A	0.9600
N2—H2	0.8600	C5—H5B	0.9600
C1—C2	1.406 (2)	C5—H5C	0.9600

C1—C5	1.485 (3)	C6—H6A	0.9600
C2—C3	1.382 (2)	C6—H6B	0.9600
C2—C4	1.497 (2)	C6—H6C	0.9600
C3—C6	1.490 (3)	O1—H1	0.8200
C4—O1	1.405 (2)		

C1—N1—N2	105.41 (13)	O1—C4—H4B	109.3
C3—N2—N1	112.18 (14)	C2—C4—H4B	109.3
C3—N2—H2	123.9	H4A—C4—H4B	108.0
N1—N2—H2	123.9	C1—C5—H5A	109.5
N1—C1—C2	110.37 (15)	C1—C5—H5B	109.5
N1—C1—C5	120.95 (16)	H5A—C5—H5B	109.5
C2—C1—C5	128.68 (16)	C1—C5—H5C	109.5
C3—C2—C1	105.41 (14)	H5A—C5—H5C	109.5
C3—C2—C4	126.49 (16)	H5B—C5—H5C	109.5
C1—C2—C4	128.08 (16)	C3—C6—H6A	109.5
N2—C3—C2	106.63 (15)	C3—C6—H6B	109.5
N2—C3—C6	122.13 (17)	H6A—C6—H6B	109.5
C2—C3—C6	131.22 (16)	C3—C6—H6C	109.5
O1—C4—C2	111.48 (14)	H6A—C6—H6C	109.5
O1—C4—H4A	109.3	H6B—C6—H6C	109.5
C2—C4—H4A	109.3	C4—O1—H1	109.5

C1—N1—N2—C3	0.1 (2)	N1—N2—C3—C6	−179.26 (17)
N2—N1—C1—C2	0.16 (19)	C1—C2—C3—N2	0.42 (19)
N2—N1—C1—C5	−178.96 (16)	C4—C2—C3—N2	−178.21 (15)
N1—C1—C2—C3	−0.37 (19)	C1—C2—C3—C6	179.2 (2)
C5—C1—C2—C3	178.66 (18)	C4—C2—C3—C6	0.6 (3)
N1—C1—C2—C4	178.24 (15)	C3—C2—C4—O1	−84.9 (2)
C5—C1—C2—C4	−2.7 (3)	C1—C2—C4—O1	96.7 (2)
N1—N2—C3—C2	−0.3 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.98	2.7965 (18)	177
N2—H2···O1^{ii}	0.86	1.98	2.842 (2)	179

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2.

Fig. 1