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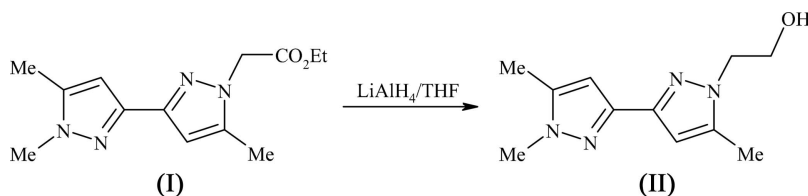
## Key indicators

Single-crystal X-ray study  
 $T = 173$  K  
Mean  $\sigma(C-C) = 0.003$  Å  
 $R$  factor = 0.049  
 $wR$  factor = 0.125  
Data-to-parameter ratio = 14.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 2-(1',5',5-Trimethyl-3,3'-bi-1H-pyrazol-1-yl)ethanol

In the crystal structure of the title compound,  $C_{11}H_{16}N_4O$ , the two pyrazole rings are coplanar, as indicated by both the dihedral angle of  $0.8(1)^\circ$  between their mean planes and the  $N-C-C-N$  torsion angle of  $179.81(13)^\circ$ .Received 7 March 2006  
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## Comment

Pyrazole derivatives are of particular interest in coordination chemistry. Several pyrazole-containing compounds have shown ability to complex transition metal ions (Jeong *et al.*, 2003; Bol *et al.*, 1997; Mary *et al.*, 1993; Elguero *et al.*, 1980). However, the literature reports few applications of *C,C*-bipyrazole derivatives in coordination chemistry. In this paper, we have synthesized and determined the X-ray crystal structure of a new *C,C*-bipyrazole ligand, (1',5',5-trimethyl-3,3'-bi-1H-pyrazol-1-yl)ethanol, (II), functionalized with a mobile chain containing a donor heteroatom. Ligand (II) was prepared by reduction of (1',5',5-trimethyl-3,3'-bi-1H-pyrazol-1-yl)ethyl acetate, (I), by  $LiAlH_4$ ; it has two pyrazole  $Nsp^2$  atoms and one O atom at the end of a flexible side chain.The pyrazole-to-methyl bond lengths  $C11-C12$  and  $C5-C6$  (Table 1) are very close to those observed in 1-(*p*-nitrophenyl)-3-methyl-4-bromopyrazole (Lapasset & Falgueirettes, 1972). The  $N1-N2$  and  $N3-N4$  bond lengths are within the values [ $1.2348(8)$ – $1.385(4)$  Å] reported for  $N-N$  bonds in pyrazole rings (Krishna *et al.*, 1999).The atoms of the pyrazole rings do not deviate from their least-squares mean planes by more than  $0.0018(9)$  Å (atoms  $N1$  and  $C8$ ). These deviations may be compared with that ( $0.012$  Å for  $C6$ ) in 1-(*p*-nitrophenyl)-3-methyl-4-bromopyrazole (Lapasset & Falgueirettes, 1972).With a  $N1-C8-C9-N3$  torsion angle of  $179.81(13)^\circ$ , the two heterocycles are coplanar and their N atoms are *trans* with respect to the  $C8-C9$  bond. This configuration has already been observed in the 3,3'-bipyrazole (Monge *et al.*, 1994). Electron delocalization and conjugation in the pyrazole  $\pi$  systems may occur between the two rings. This is indicated by the shortening of the  $C8-C9$  bond length to  $1.463(2)$  Å [ $1.4586$  Å in the 3,3'-bipyrazole (Monge *et al.*, 1994)] and also by the small dihedral angle of  $0.8(1)^\circ$  between the pyrazole mean planes.

The low steric hindrance between substituents at positions 1 (or 1') and 5 (or 5') results in small values of 2.7 (2) and 0.4 (2)°, respectively, for the C13–N4–C11–C12 and C6–C5–N2–C3 torsion angles.

In the crystal structure, molecules of (II) form hydrogen-bonded centrosymmetric dimers through O–H···N bonds (Table 2).

## Experimental

Bipyrazole (I) (0.63 g, 2.40 mmol) dissolved in tetrahydrofuran (THF, 20 ml) was added to a stirred suspension of LiAlH<sub>4</sub> (200 mg, 5.26 mmol) in THF (10 ml) cooled to 273 K. The mixture was stirred under reflux for 2 h. After cooling to 273 K, the excess hydride was destroyed by slow addition of water (0.2 ml), aqueous sodium hydroxide (15%, 0.2 ml) and then water (0.6 ml). The stirring was continued for 2 h, the solid material filtered off and the residue washed with hot THF. The filtrate and THF washings were concentrated under reduced pressure and the resulting solid was recrystallized from THF as colourless crystals of (II) suitable for X-ray analysis (yield 72%; m.p. 451–453 K).

### Crystal data

C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> O	$V = 549.2 (1) \text{ \AA}^3$
$M_r = 220.28$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.332 \text{ Mg m}^{-3}$
$a = 6.9135 (7) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 7.3389 (8) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 12.183 (1) \text{ \AA}$	$T = 173 (2) \text{ K}$
$\alpha = 86.09 (1)^\circ$	Parallelepiped, colourless
$\beta = 82.18 (1)^\circ$	$0.35 \times 0.30 \times 0.12 \text{ mm}$
$\gamma = 63.75 (1)^\circ$	

### Data collection

Oxford Diffraction Xcalibur CCD diffractometer	2185 independent reflections
$\omega$ scans	1797 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.077$
7672 measured reflections	$\theta_{\text{max}} = 26.1^\circ$

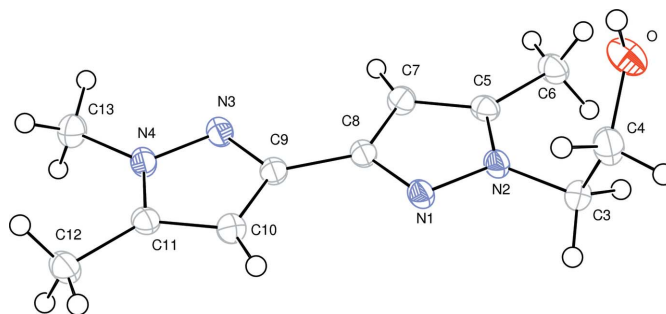
### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.2622P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.125$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
2185 reflections	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
152 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

N1–N2	1.3650 (18)	N4–C13	1.455 (2)
N2–C3	1.460 (2)	C12–C11	1.494 (2)
N3–N4	1.3595 (19)	C5–C6	1.491 (2)
C8–C9	1.463 (2)		
N1–C8–C9–N3	179.81 (13)	C3–N2–C5–C6	0.4 (2)
N3–N4–C11–C12	–178.96 (13)		



**Figure 1**

View of (II). Displacement ellipsoids for the non-H atoms are drawn at the 30% probability level.

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O-H\cdots N1^i$	0.87 (3)	2.10 (3)	2.9441 (19)	162 (2)

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

Except for the hydroxy H atom, which was located in a Fourier difference map and whose position and isotropic displacement parameter were freely refined, all H atoms were placed in geometrically idealized positions ( $C-H = 0.93\text{--}0.97 \text{ \AA}$ ) and constrained to ride on their parent atoms, with  $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$  for methyl groups and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$  for other H atoms.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Version 1.08; Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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