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Key indicators

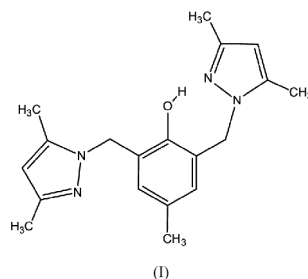
Single-crystal X-ray study
T = 183 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.078
wR factor = 0.142
Data-to-parameter ratio = 14.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

2,6-Bis(3,5-dimethylpyrazol-1-ylmethyl)-4-methylphenol

The crystal structure of the title compound, $\text{C}_{19}\text{H}_{24}\text{N}_4\text{O}$, has been determined in the monoclinic space group $P2_1/c$. The two pyrazole substituents are arranged *trans* to each other; the dihedral angle between them is $83.9(1)^\circ$. There is an intramolecular hydrogen bond, with an $\text{O}\cdots\text{N}$ distance of $2.769(4) \text{ \AA}$, and an intermolecular hydrogen bond, with an $\text{O}\cdots\text{N}$ distance of $3.197(4) \text{ \AA}$.

Comment

Like other tripod multidentate ligands, the pentadentate 2,6-bis(3,5-dimethylpyrazol-1-ylmethyl)-4-methylphenol, (I), has a good capacity for coordination with transition metals ions, giving rise to chelate complexes with intense colors.



Suzuki *et al.* (1981) linked two bis(2-pyridylmethyl)amine groups to two arms of 2,6-bis(chloromethyl)-4-methylphenol, resulting in a tripod multidentate ligand, 2,6-bis[bis(2-pyridylmethyl)-amino methyl]-4-methylphenol, $\text{C}_{33}\text{H}_{34}\text{N}_6\text{O}$. In the current work, we have joined two 3,5-dimethylpyrazole groups to two arms of 2,6-bis(chloromethyl)-4-methylphenol and produced a new pentadentate ligand, (I). As the most stable configuration, the two pyrazole groups of the molecule are arranged *trans* to each other, with a dihedral angle of $83.9(1)^\circ$. The compound acts as a versatile ligand for metal ions (such as Zn^{2+}) by coordinating through pyrazole N and hydroxy O atoms after deprotonation and intramolecular rotation.

The geometric parameters of (I) are listed in Table 1, and the molecular conformation and crystal packing are illustrated in Figs. 1 and 2.

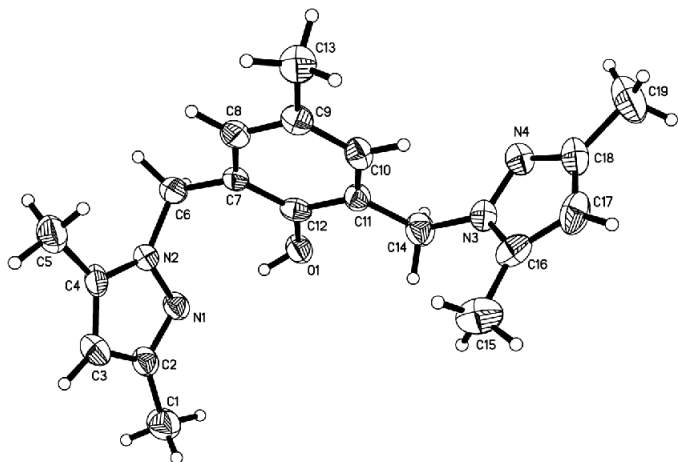
Experimental

Compound (I) was synthesized *via* a modification of the method of Kamaras *et al.* (1994). The smaller ligand, 3,5-dimethylpyrazole, which acts as the chelating arm in the target compound, was prepared according to the method of Wiley & Hexner (1963). To a solution of 3,5-dimethylpyrazole in dimethylformamide, containing NaH, was added dropwise 2,6-bis(chloromethyl)-4-methylphenol, with vigorous stirring at room temperature (yield 80%; m.p. 398 K). 2,6-Bis[1-(3,5-

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**Figure 1**

A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

dimethyl)pyrazolemethyl]-4-methylphenol (100 mg) was dissolved in CHCl_3 (2 ml), and the solution was allowed to evaporate slowly over several days. Brown crystals suitable for X-ray diffraction were collected once all of the solution had evaporated.

Crystal data

$\text{C}_{19}\text{H}_{24}\text{N}_4\text{O}$
 $M_r = 324.42$
 Monoclinic, $P2_1/c$
 $a = 9.508$ (3) Å
 $b = 18.747$ (6) Å
 $c = 10.116$ (3) Å
 $\beta = 105.085$ (5)°
 $V = 1741.0$ (9) Å³
 $Z = 4$

$D_x = 1.238$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 8255 reflections
 $\theta = 2.4$ – 19.6 °
 $\mu = 0.08$ mm⁻¹
 $T = 183$ (2) K
 Slab, colorless
 $0.2 \times 0.2 \times 0.1$ mm

Data collection

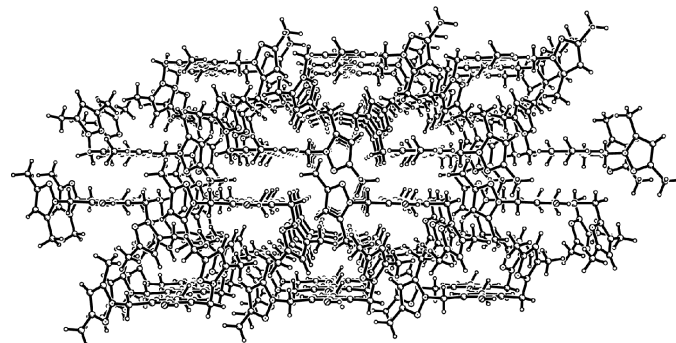
Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.984$, $T_{\max} = 0.992$
 7045 measured reflections

3053 independent reflections
 1641 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$
 $\theta_{\text{max}} = 25.0$ °
 $h = -10 \rightarrow 11$
 $k = -22 \rightarrow 17$
 $l = -11 \rightarrow 12$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.078$
 $wR(F^2) = 0.142$
 $S = 0.98$
 3053 reflections
 217 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0393P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

**Figure 2**

The crystal packing of (I), viewed down the b axis.

Table 1

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}$	0.84	1.95	2.769 (4)	163
$\text{O1}-\text{H1}\cdots\text{N2}$	0.84	2.56	3.197 (4)	133

All H atoms were initially located in a difference Fourier map. They were then constrained to be riding, with $C-H = 0.98$ – 1.00 Å and $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$ of the parent atom.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000) and *SHELXTL/PC* (Sheldrick, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *SHELXTL/PC*.

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