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2,6-Bis(imidazol-1-ylmethyl)-4-methylphenol monohydrate

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.052
wR factor = 0.150
Data-to-parameter ratio = 13.3

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

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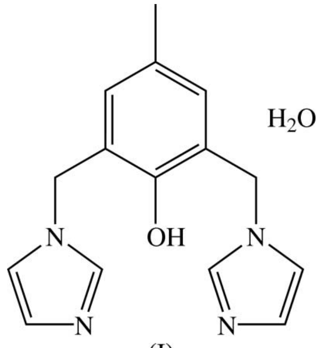
In the title compound, $C_{15}H_{16}N_4O\cdot H_2O$, the two imidazole rings adopt a *trans* conformation with respect to the phenol plane. A hydrogen-bonded two-dimensional supramolecular network exists in the crystal structure.

Comment

The title compound, (I), is a multidentate ligand. The present X-ray single-crystal diffraction experiment revealed that it crystallizes as a monohydrate. The molecular structure of (I) with the atom-numbering scheme is shown in Fig. 1.



(I)

The bond distances and angles of the benzene ring, the imidazole rings and the methyl group in this structure are in normal ranges (Chu *et al.*, 2005; Xu *et al.*, 2005).

The two imidazole rings adopt a *trans* conformation with respect to the phenol plane. The angles between the planes of

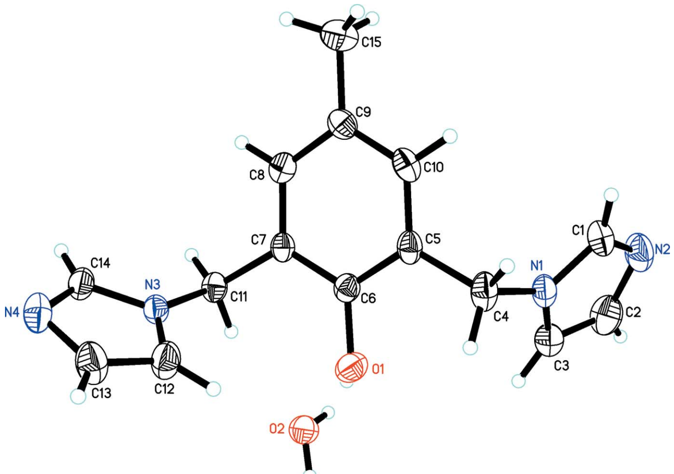


Figure 1
A drawing of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

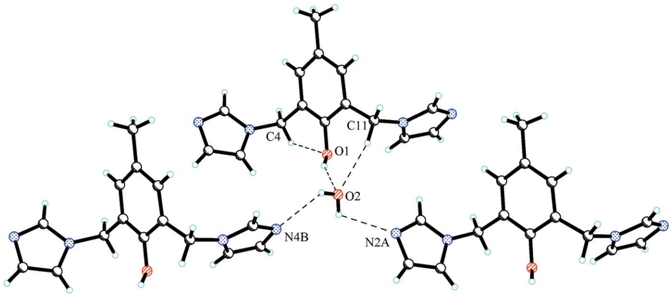


Figure 2
A perspective view of the hydrogen bonds around the solvent water molecule [symmetry codes: (A) $x, -1 + y, z$; (B) $-1 + x, y, z$]. Hydrogen bonds are shown as dashed lines.

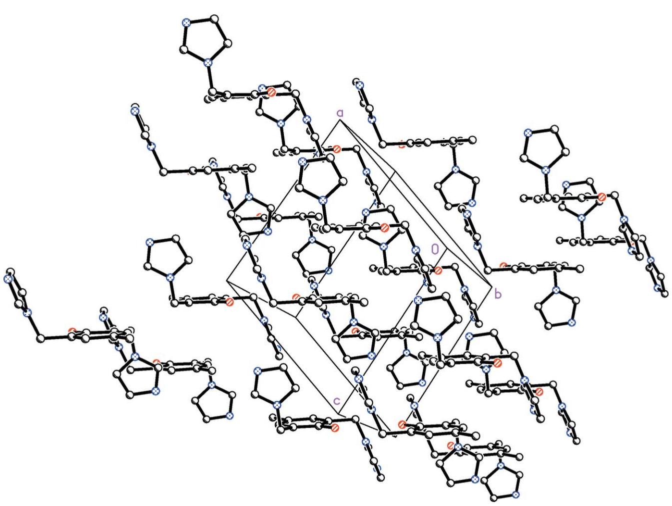


Figure 3
A packing diagram of (I), showing that all the benzene rings in the unit cell are parallel to one another. The water molecules and H atoms have been omitted for clarity.

the phenol ring and imidazole rings *A* (atoms C1–C3/N1/N2) and *B* (atoms C12–C14/N3/N4) are 70.5 (2) and 104.1 (2)°, respectively, with the two imidazole rings inclined at 93.5 (2)° to each other. The structure is different from that which we recently reported, *viz*. 4-*tert*-butyl-2,6-bis[(imidazolium-1-yl)methyl]phenol tetrachlorozincate(II) [(II); Xu *et al.*, 2005], in which the two imidazole rings are *cis* relative to the phenol plane.

The hydrogen-bonding interactions are the most notable intermolecular feature in (I). The solvent water molecules are linked to three adjacent molecules. These links comprise one O—H···O hydrogen bond with the phenolic H atom, two O—H···N hydrogen bonds with imidazole atoms N2 and N4, and one C—H···O hydrogen bond with a methylene H atom bound to C11 (Fig. 2). In addition, there is one intramolecular C—H···O hydrogen bond between phenol atom O1 and a methylene H atom bonded to C4. These hydrogen bonds form the framework of a two-dimensional network.

All the phenol rings are parallel to one another in the crystal packing of (I), as illustrated in Fig. 3. Although they are parallel, there are no π–π stacking interactions between the aromatic rings. This is also seen in the structure of (II).

Experimental

The title compound, (I), was prepared *via* a one-step Mannich reaction as a white powder in 57% yield (Yan *et al.*, 1994). Colourless single crystals suitable for X-ray analysis were grown from a mixture of ethanol and water in a 2:1 (*v*/*v*) ratio by slow evaporation at room temperature in air.

Crystal data

$C_{15}H_{16}N_4O \cdot H_2O$
$M_r = 286.33$
Triclinic, $P\overline{1}$
$a = 8.802$ (1) Å
$b = 9.606$ (2) Å
$c = 10.648$ (2) Å
$\alpha = 105.46$ (1)°
$\beta = 105.34$ (1)°
$\gamma = 112.33$ (1)°
$V = 732.0$ (3) Å^3

$Z = 2$
$D_x = 1.299$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1249 reflections
$\theta = 2.5$–24.9°
$\mu = 0.09$ mm^{-1}
$T = 291$ (2) K
Block, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.984$, $T_{max} = 0.990$
3699 measured reflections

2544 independent reflections
1791 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 25.0°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 11$
$l = -7 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.151$
$S = 1.00$
2544 reflections
191 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0874P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C4—N1	1.462 (3)	C7—C11	1.507 (3)
C4—C5	1.512 (3)	C11—N3	1.466 (3)
N1—C4—C5	112.41 (18)	N3—C11—C7	111.71 (18)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*B*···O2	0.97	2.38	3.314 (3)	162
C4—H4*B*···O1	0.97	2.40	2.802 (3)	104
O2—H2*C*···N4^{i}	0.85	2.34	2.824 (2)	117
O2—H2*A*···N2^{ii}	0.85	2.43	2.788 (3)	106
O1—H1*B*···O2	0.96	1.79	2.668 (2)	151

Symmetry codes: (i) $x - 1, y, z$; (ii) $x, y - 1, z$.

H atoms were placed in geometrically idealized positions (C—H = 0.93–0.97 Å and O—H = 0.85–0.96 Å) and refined as riding atoms, with $U_{iso}(H) = 1.5U_{eq}$(O and methyl C) or $1.2U_{eq}$(C) for all other C atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine

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structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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