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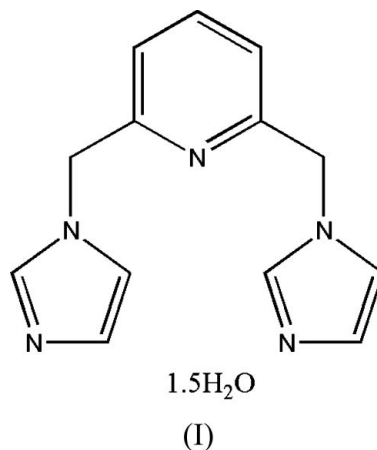
## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.049  
 $wR$  factor = 0.148  
Data-to-parameter ratio = 15.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2,6-Bis(1*H*-imidazol-1-ylmethyl)pyridine  
sesquihydrate

The title compound,  $\text{C}_{13}\text{H}_{13}\text{N}_5 \cdot 1.5\text{H}_2\text{O}$ , was synthesized by the reaction of 2,6-bis(bromomethyl)pyridine with imidazole. The asymmetric unit contains two crystallographically independent 2,6-bis(1*H*-imidazol-1-ylmethyl)pyridine molecules and three water molecules. The crystal packing is stabilized by  $\text{O} \cdots \text{O}$  and  $\text{O}-\text{H} \cdots \text{N}$  hydrogen-bond interactions.

## Comment

In recent years, many *N*-heterocyclic carbene cyclophanes have been synthesized and studied for their capability to act as molecular recognition reagents in host-guest systems (Herrmann & Köcher, 1997; Bourissou *et al.*, 2000; Lee *et al.*, 2004; Yoon *et al.*, 2004). As a continuation of our systematic studies of various *N*-heterocyclic carbene ligands, the title compound, (I), has been synthesized and its crystal structure is reported here.



The asymmetric unit of (I) contains two crystallographically independent organic molecules (molecule *A*: N1–N5/C1–C13; molecule *B*: N6–N10/C14–C26) and three water molecules (Fig. 1). The geometry of the two molecules is similar, the main difference being the orientation of the N5/N10/C24/C25/C26 imidazole ring; in molecule *B* this is rotated by about 180° around the N5–C23 bond with respect to the corresponding N1/N2/C1/C2/C3 ring in molecule *A*. The dihedral angles between the imidazole rings are 77.99 (11) and 76.63 (11)° in molecules *A* and *B*, respectively. The dihedral angles formed by the pyridine ring with the imidazole rings are 78.17 (9) and 68.39 (9)° (molecule *A*) and 80.03 (9) and 70.83 (7)° (molecule *B*).

In the crystal structure, there are  $\text{O}-\text{H} \cdots \text{O}$  and  $\text{O}-\text{H} \cdots \text{N}$  hydrogen-bonding interactions involving the water molecules (Table 1).

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## Experimental

The title compound was prepared according to a literature method (Garrison *et al.*, 2001). Imidazole (6.8 g, 100 mmol) in THF (20 ml) was added dropwise to KH (4.0 g, 100 mmol) in THF (20 ml) while stirring at room temperature. Stirring was continued for 16 h. To this slurry 1,3-bis(bromomethyl)pyridine (13.3 g, 50 mmol) was added and the resulting solution was stirred for an additional 18 h. The solution was filtered and the volatile materials were removed under reduced pressure to yield (I) as an off-white solid. Single crystals suitable for X-ray analysis were obtained by slow evaporation of a toluene solution.

### Crystal data

$C_{13}H_{13}N_5 \cdot 1.5H_2O$   
 $M_r = 266.31$   
 Triclinic,  $P\bar{1}$   
 $a = 9.260$  (2) Å  
 $b = 10.846$  (3) Å  
 $c = 15.531$  (4) Å  
 $\alpha = 77.794$  (4)°  
 $\beta = 87.324$  (4)°  
 $\gamma = 65.873$  (4)°  
 $V = 1390.0$  (6) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.273$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1781 reflections  
 $\theta = 2.3$ – $25.8$ °  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 Block, colourless  
 $0.22 \times 0.20 \times 0.16$  mm

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1999)  
 $T_{\min} = 0.972$ ,  $T_{\max} = 0.986$   
 7869 measured reflections

5600 independent reflections  
 2796 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 26.4$ °  
 $h = -11 \rightarrow 11$   
 $k = -9 \rightarrow 13$   
 $l = -19 \rightarrow 17$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.149$   
 $S = 1.01$   
 5600 reflections  
 370 parameters  
 H atoms treated by a mixture of independent and constrained refinement

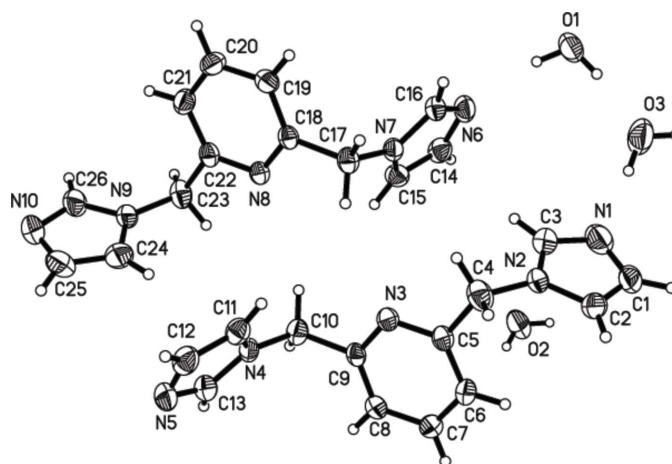
$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 0.1192P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.17$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.18$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1A \cdots O3$	0.88 (1)	1.78 (1)	2.644 (3)	166 (3)
$O1-H1B \cdots N6$	0.86 (2)	2.03 (1)	2.872 (2)	165 (2)
$O2-H2A \cdots O1^i$	0.86 (2)	2.01 (1)	2.864 (3)	171 (3)
$O2-H2B \cdots N5^{ii}$	0.87 (3)	2.12 (1)	2.975 (3)	169 (3)
$O3-H3A \cdots N10^{iii}$	0.86 (1)	1.86 (1)	2.717 (3)	174 (3)
$O3-H3B \cdots N1$	0.86 (3)	1.97 (2)	2.797 (3)	162 (4)

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



**Figure 1**

The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids.

The H atoms of the water molecules were found in a difference electron-density map and refined freely. All other H atoms were included at their idealized positions, and allowed to ride on their parent atoms, with  $C-H = 0.93$ – $0.97$  Å and  $U_{\text{iso}} = 1.2U_{\text{eq}}(C)$ .

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); 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, 1999); software used to prepare material for publication: SHELXTL.

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