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trans-1,2-Bis(4-pyridyl)ethylene monohydrate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.090
Data-to-parameter ratio = 8.3

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

In the title compound, $C_{12}H_{10}N_2\cdot H_2O$, intermolecular O—H···N hydrogen bonds are highly effective in forming a one-dimensional chain. In addition, the presence of C—H···O hydrogen bonds helps to build a three-dimensional supramolecular network, thereby stabilizing the crystal structure.

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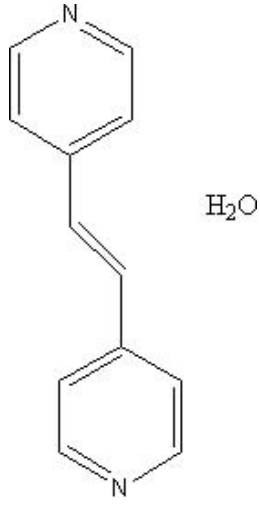
Comment

1,2-Bis(4-pyridyl)ethylene is a bidentate ligand in terms of coordination chemistry and to date a large number of structures involving this molecule have been reported. Both *cis* and *trans* isomers have been structurally characterized (Wenger *et al.*, 2004; Vansant *et al.*, 1980). In this paper, we present the crystal structure of the *trans* isomer in its monohydrate form, (I).



(I)

The atom-numbering scheme of (I) is shown in Fig. 1, while selected bond distances and bond angles are given in Table 1. The molecule adopts a *trans* configuration, with a dihedral angle between the pyridine rings of 20.3 (2)°.

Intermolecular hydrogen-bonding interactions are the most important feature in the title compound. O—H···N hydrogen

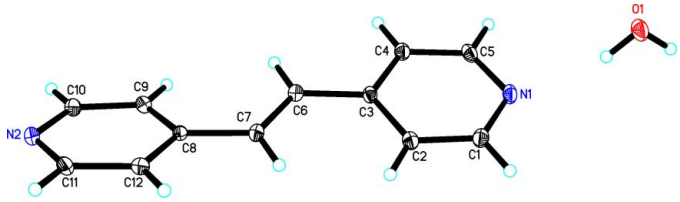


Figure 1
The title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

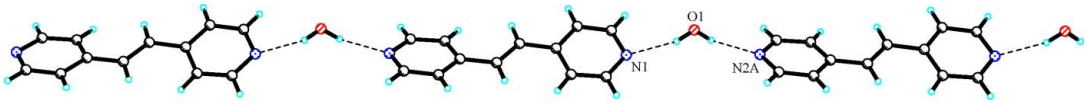


Figure 2
View of the one-dimensional chain structure sustained by hydrogen bonds (dashed lines). Suffix A denotes symmetry operator (x, $1 + y$, z).

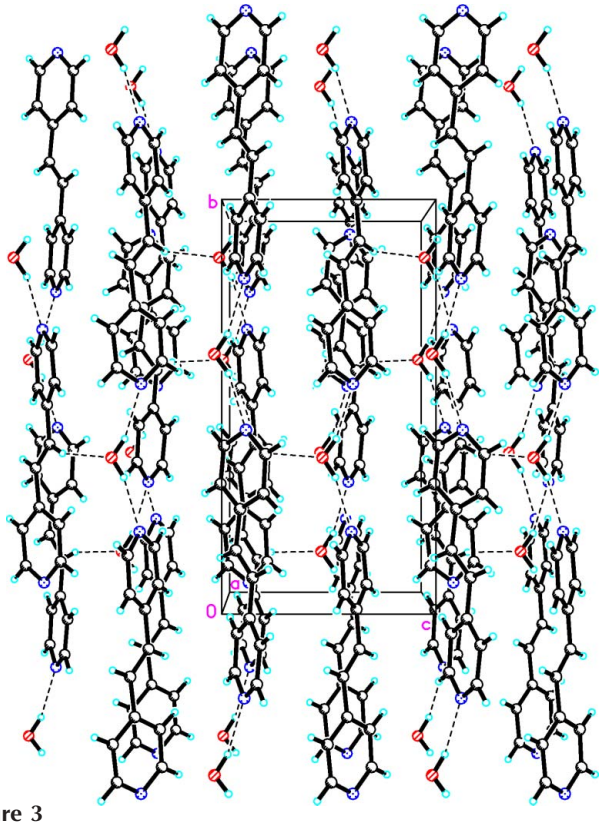


Figure 3
Packing diagram of (I), viewed along the a axis. Dashed lines indicate hydrogen bonds.

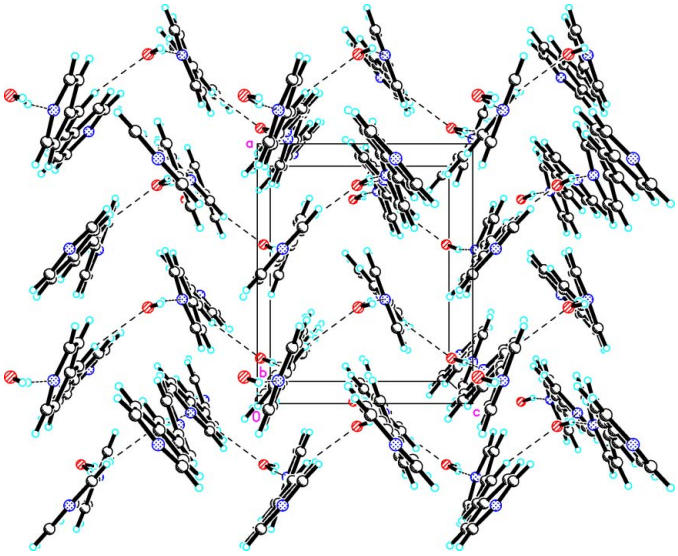


Figure 4
Perspective view of (I), viewed along the b axis. Dashed lines indicate hydrogen bonds.

bonds between the N atoms of adjacent pyridine rings and the water molecules link the *trans*-1,2-bis(4-pyridyl)ethylene molecules into one-dimensional chains extending along the b axis (Fig. 2 and Table 2). Neighboring chains are packed *via* van der Waals interactions; there are no π–π stacking interactions between the aromatic rings (Fig. 3). In addition, the structure is further stabilized by weak C—H···O hydrogen bonds between the H atom bonded to C7 and the water molecule, forming a three-dimensional supramolecular hydrogen-bond network (Fig. 4).

Experimental

trans-1,2-Bis(4-pyridyl)ethylene was purchased from Aldrich Co. Colorless crystals suitable for X-ray analysis were grown from a mixture of ethanol and water (3:1) by slow evaporation at room temperature. Analysis calculated for $C_{12}H_{12}N_2O$: C 71.98, N 13.99, H 6.04%; found: C 71.96, N 13.98, H,6.07%.

Crystal data

$C_{12}H_{10}N_2\cdot H_2O$
$M_r = 200.24$
Orthorhombic, $Pna2_1$
$a = 9.1778\ (18)$ Å
$b = 14.768\ (3)$ Å
$c = 7.6109\ (15)$ Å
$V = 1031.5\ (4)$ Å^3
$Z = 4$
$D_x = 1.289$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4671 reflections
$\theta = 3.5$–$27.5°$
$\mu = 0.08$ mm^{-1}
$T = 100\ (2)$ K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
$T_{min} = 0.978$, $T_{max} = 0.982$
9337 measured reflections
1194 independent reflections
1182 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 27.0°$
$h = -11 \rightarrow 11$
$k = -18 \rightarrow 15$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.090$
$S = 1.17$
1194 reflections
144 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.2772P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.339 (3)	C7—C8	1.474 (2)
C3—C6	1.482 (2)	C10—N2	1.341 (3)
C5—N1	1.336 (3)	C11—N2	1.338 (3)
C6—C7	1.333 (3)		
C7—C6—C3	124.08 (17)	C6—C7—C8	125.35 (17)
C2—C3—C6—C7	2.5 (3)	C6—C7—C8—C9	17.1 (3)
C3—C6—C7—C8	−178.96 (19)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.95	2.39	3.284 (3)	157
O1—H1B···N2^{ii}	0.87 (5)	2.05 (5)	2.875 (2)	159 (4)
O1—H1A···N1	0.85 (4)	2.08 (4)	2.897 (2)	161 (4)

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

H atoms, except those of the water molecule, were placed in geometrically idealized positions (C—H = 0.95 Å) and refined as riding atoms, with U_{iso}(H) = 1.2$_{eq}$(C). Water H atoms were located in a difference synthesis map and refined isotropically [O—H = 0.85 (4)–0.87 (5) Å]. In the absence of significant anomalous scattering, Friedel equivalents were merged before the final refinement.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku Corporation, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku Corporation, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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