

1-(6-Bromopyridin-2-yl)-3-methyl-3*H*-imidazol-
1-ium bromide monohydratePi Yun Cheng, Jing Yao Zeng,
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The structure of the title compound, $C_9H_9BrN_3^+ \cdot Br^- \cdot H_2O$, was determined at 150 K. It is a supramolecular adduct of imidazolium bromide and water molecules. Helical chains of $(H_2O \cdot Br^-)$ exist in the structure along the [001] direction. Each chain forms extensive hydrogen bonds with the imidazolium cations.

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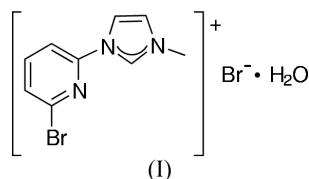
Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(C-C) = 0.007$ Å
 R factor = 0.035
 wR factor = 0.097
Data-to-parameter ratio = 19.8

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

Comment

N-Heterocyclic carbene (NHC) ligands are attracting much research attention for their wide applicability in coordination chemistry and catalysis. They are generally accessible by deprotonation of the corresponding imidazolium salts. Our current research effort is focused on synthesizing novel chelating ligands based on NHC and investigating their catalytic properties (Lee *et al.*, 2004, 2005). In the course of preparing a pyridine-functionalized NHC precursor, we isolated the title imidazolium salt, (I).



We present here the structure of (I) (Fig. 1). It crystallizes in the non-centrosymmetric orthorhombic space group $Pna2_1$ with a water molecule incorporated in the asymmetric unit.

The incorporated water molecules and Br^- anions form helical chains along the [001] direction (Fig. 2). Each chain forms extensive hydrogen bonds of the types $C-H \cdots Br$ and $C-H \cdots O$ with the imidazolium cations (Table 1 and Fig. 3).

Experimental

The title compound was isolated from a mixture of *N*-methylimidazole and 2,6-dibromopyridine heated at 393 K for 2 d. Crystals were grown by slow diffusion of diethyl ether into a dimethylformamide solution of the compound.

Crystal data

$C_9H_9BrN_3^+ \cdot Br^- \cdot H_2O$
 $M_r = 337.03$
Orthorhombic, $Pna2_1$
 $a = 7.1233$ (3) Å
 $b = 17.3399$ (7) Å
 $c = 9.5533$ (4) Å
 $V = 1180.00$ (8) Å³
 $Z = 4$
 $D_x = 1.897$ Mg m⁻³

Mo $K\alpha$ radiation
Cell parameters from 4258 reflections
 $\theta = 2.3$ – 27.8°
 $\mu = 6.85$ mm⁻¹
 $T = 150$ (2) K
Block, colorless
 $0.23 \times 0.18 \times 0.16$ mm

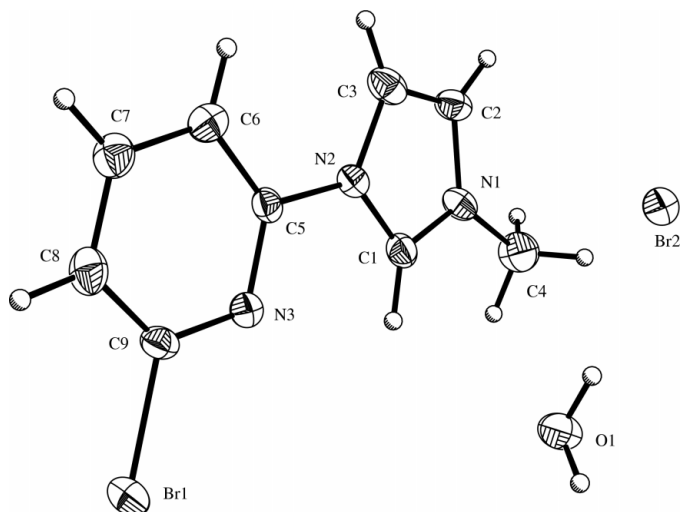


Figure 1
The structure of (I), showing 50% displacement ellipsoids for the non-H atoms.

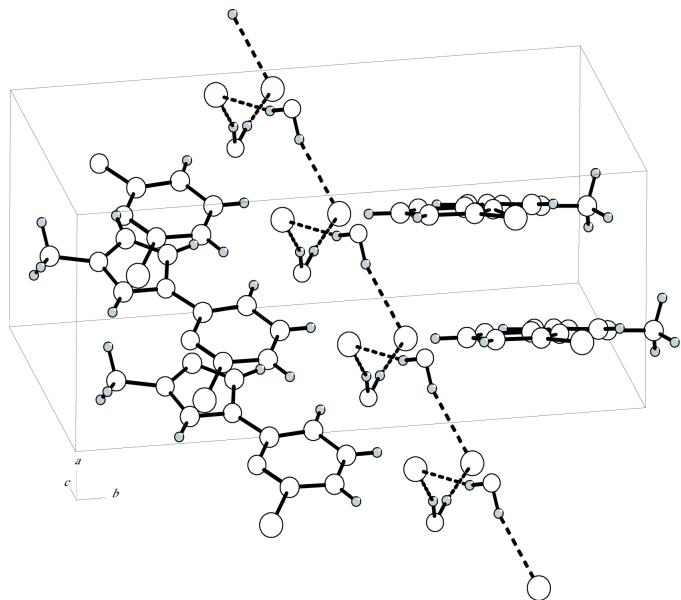


Figure 2
A view of the packing, showing the hydrogen-bonded (dashed lines) helical chain of water molecules and bromide anions.

Data collection

Bruker SMART APEX-II diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.237$, $T_{\max} = 0.334$
 11417 measured reflections

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.097$
 $S = 1.05$
 2877 reflections
 145 parameters
 H-atom parameters constrained

2877 independent reflections
 2522 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.047$
 $\theta_{\text{max}} = 28.7^\circ$
 $h = -9 \rightarrow 9$
 $k = -23 \rightarrow 23$
 $l = -12 \rightarrow 11$

$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.84 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.64 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983),
 1258 Friedel pairs
 Flack parameter = 0.042 (16)

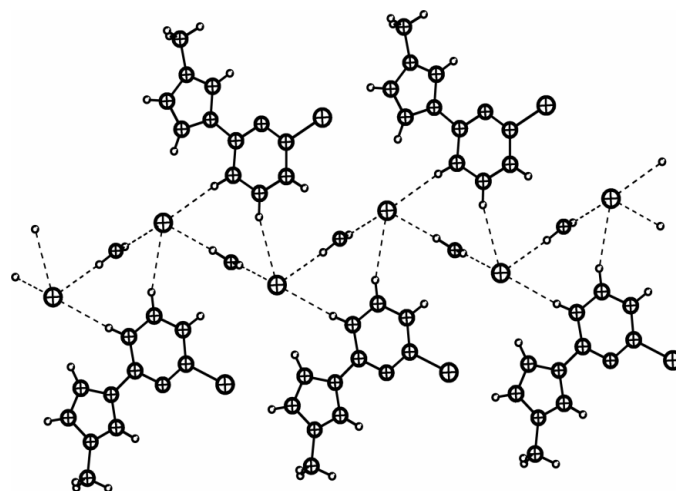


Figure 3
A view of the packing of (I), showing the hydrogen-bonding network (dashed lines).

Table 1
Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H11 \cdots Br2	0.96 (10)	2.38 (10)	3.324 (4)	165 (6)
C1—H1 \cdots O1	0.95	2.66	3.196 (6)	116
C3—H3 \cdots Br2 ⁱ	0.95	2.91	3.847 (6)	168
C6—H6 \cdots Br2 ⁱ	0.95	2.83	3.771 (5)	173
C8—H8 \cdots O1 ⁱⁱ	0.95	2.54	3.431 (7)	156
C7—H7 \cdots Br2 ⁱⁱ	0.95	2.85	3.768 (5)	162
C4—H4B \cdots O1 ⁱⁱⁱ	0.98	2.66	3.327 (8)	125
C2—H2 \cdots O1 ⁱⁱⁱ	0.95	2.62	3.375 (6)	136
C4—H4C \cdots Br1 ⁱⁱⁱ	0.98	3.03	3.667 (6)	124

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

Atoms H10 and H11 are located from the difference map and refined isotropically. Other H atoms were positioned geometrically and refined with a riding model, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ for all other H atoms.

Data collection: APEX2 (Bruker, 2001) and SMART (Bruker, 2001); cell refinement: APEX2 and SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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