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1-Ethyl-2,3-dimethylimidazolium bromide monohydrate

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The asymmetric unit of the title compound, $C_7H_{11}N_2^+\cdot Br^-\cdot H_2O$, consists of one crystallographically independent 1-ethyl-2,3-dimethylimidazolidinium cation, one bromide anion and one water molecule, all of them located in general positions. In the crystal structure, the bromide anions and the water molecules are connected *via* O—H···Br hydrogen bonding to form dimers which are located on centres of inversion. In addition, the cations are connected to the water molecules *via* weak C—H···O hydrogen bonding.

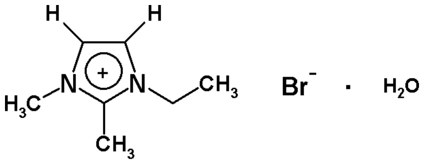
Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.007 Å
R factor = 0.054
wR factor = 0.168
Data-to-parameter ratio = 23.8

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

Comment

In order to study the effect of hydrogen bonding on the structures of ionic liquid compounds, we have synthesized substituted imidazolium bromides. We report here the crystal structure of 1-ethyl-2,3-dimethylimidazolium bromide monohydrate, (I), at room temperature. The structure is built up by double chains of planar imidazolium rings running along the crystallographic *a* axis (Fig. 1).



(I)

The ethyl group deviates from the aromatic ring plane. The torsion angles are C2—N1—C6—C7 = −93.1 (6)° and C5—

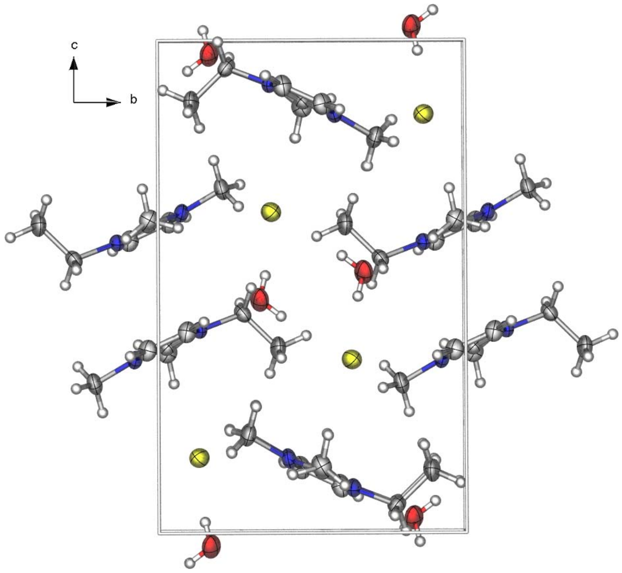


Figure 1
The crystal structure of (I), viewed along the *a* axis.

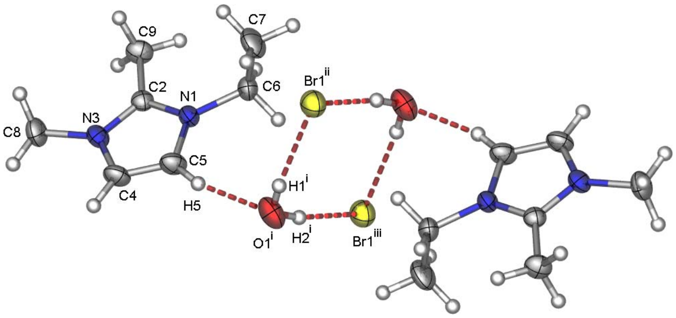


Figure 2
Part of the crystal structure of (I), showing the atom labelling and the C—H$\cdots$O and O—H$\cdots$Br hydrogen bonding (dashed lines). [Symmetry codes: (i) $x-1, y, z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (iii) $\frac{1}{2}+x, \frac{3}{2}-y, -\frac{1}{2}+z$.]

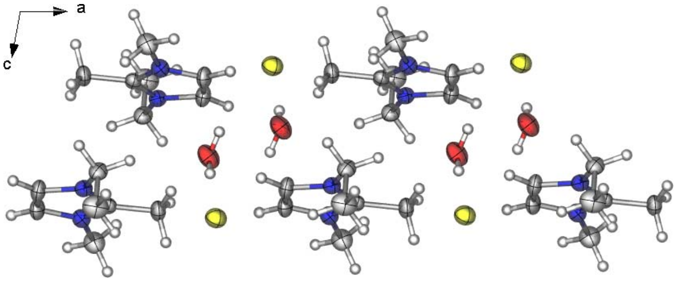


Figure 3
The crystal structure of (I), viewed along the *b* axis, showing the arrangement of the cations.

N1—C6—C7 = 82.9 (6)°. Coplanar with the cationic heterocycles, solvent water molecules are incorporated, while the anions fill the remaining space between the ring planes (see Fig. 1). Atom O1 is involved in hydrogen bonding with H5 of the aromatic cation, while the bromide anion interacts with the water H atoms (Fig. 2 and Table 1). The H$\cdots$Br distances are in the expected range for hydrogen bonds derived from interactions between bromide anions and water molecules (Steiner, 2002). From Fig. 3 it is obvious that the π systems of the cations are not stacked with respect to each other. Two cations are rotated by 180° relative to each other in such a way that one of the methyl H atoms bound to methyl atom C9 of one cation is oriented in the direction of the π system of the second. From the analogous anhydrous compound 1-allyl-2,3-dimethylimidazolium bromide, it is known that the ring planes are stacked pairwise along the *b* axis, showing interplanar distances of 3.35 Å (Kölle & Dronskowski, 2004). However, in the title compound, the interplanar distance of 4.669 (7) Å is too large for significant π-stacking.

Experimental

The ionic liquid compound was prepared following modified literature procedures (Krumm & Giernoth, 2004). 1,2-Dimethylimidazole (3.37 g, 35 mmol) was dissolved in acetonitrile (50 ml) and heated to 353 K with vigorous stirring, then ethyl bromide (3.82 g, 35 mmol) was added dropwise. The reaction mixture was refluxed for 12 h at 363 K. Subsequently, the solvent was removed by distillation and the white product dried in vacuum (yield: 5.63 g, 82%). By dissolving the compound in dichloromethane and quasi-isothermic evaporation of the solvent, white crystals of the title compound were obtained.

Crystal data

$C_7H_{13}N_2^+\cdot Br^-\cdot H_2O$
$M_r = 223.12$
Monoclinic, $P2_1/n$
$a = 7.388$ (2) Å
$b = 9.2652$ (15) Å
$c = 15.117$ (4) Å
$\beta = 100.37$ (3)°
$V = 1017.9$ (4) Å^3
$Z = 4$
$D_x = 1.456$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1493 reflections
$\theta = 0$–23.2°
$\mu = 3.99$ mm^{-1}
$T = 293$ (2) K
Irregular fragment, colourless
0.5 × 0.3 × 0.2 mm

Data collection

Stoe IPDS-I diffractometer
φ scans
Absorption correction: numerical [*X-RED32* (Stoe & Cie, 2001) and *X-SHAPE* (Stoe & Cie, 1999)]
$T_{min} = 0.251$, $T_{max} = 0.455$
11 811 measured reflections
2454 independent reflections
1550 reflections with $I > 2\sigma(I)$
$R_{int} = 0.078$
$\theta_{max} = 28.1°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.168$
$S = 1.05$
2454 reflections
103 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.099P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots$O1^{i}	0.95	2.39	3.321 (6)	168
O1—H1$\cdots$Br1^{ii}	0.82	2.52	3.337 (4)	174
O1—H2$\cdots$Br1^{iii}	0.82	2.52	3.309 (4)	163

Symmetry codes: (i) $x-1, y, z$; (ii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii) $\frac{1}{2}+x, \frac{3}{2}-y, z-\frac{1}{2}$.

Carbon-bound H atoms were positioned with idealized geometry (aromatic C—H = 0.95 Å, methylene C—H = 0.99 Å and methyl C—H = 0.98 Å) and refined with fixed isotropic displacement parameters [$U_{iso}(H) = 1.5U_{eq}$(methyl C) = $1.2U_{eq}$(aromatic and methylene C)] using a riding model. The methyl group C9 was idealized (C—H = 0.98 Å), then refined as a rigid group allowed to rotate but not tip. The water H atoms were located in a difference map, their bond lengths set to ideal values (O—H = 0.82 Å), and they were refined [$U_{iso}(H) = 1.2U_{eq}(O)$] using a riding model.

Data collection: *IPDS-1 Software* (Stoe & Cie, 1996); cell refinement: *IPDS-1 Software*; data reduction: *IPDS-1 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Kölle, P. & Dronskowski, R. (2004). *Inorg. Chem.* **43**, 2803–2809.
Krumm, M. & Giernoth, R. (2004). *Adv. Synth. Catal.* **346**, 989–992.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Steiner, T. (2002) *Angew. Chem.* **102**, 50–80.
Stoe (1996). *IPDS-1 Software*. Version 2.87 (Stoe Publications 4801-007). Stoe & Cie, Darmstadt, Germany.
Stoe (1999). *X-SHAPE*. Version 1.06. Stoe & Cie, Darmstadt, Germany.
Stoe (2001). *X-RED32*. Version 1.22. Stoe & Cie, Darmstadt, Germany.