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2,3-Dimethylquinoxalinium dibromide

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Key indicators

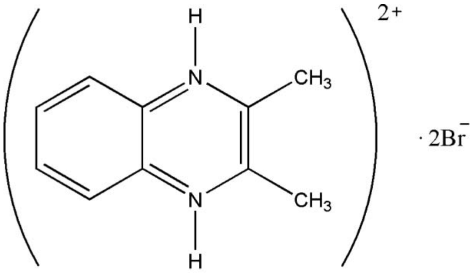
Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.019 Å
Disorder in main residue
R factor = 0.069
wR factor = 0.191
Data-to-parameter ratio = 18.3

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

The title compound, $C_{10}H_{12}N_2^{2+}\cdot 2Br^-$, crystallizes with both the cation and the two Br^- anions lying on a crystallographic mirror plane. In the crystal structure, the anions and cations are linked by N—H···Br and C—H···Br hydrogen bonds, forming a layer-like structure. The layers are stacked in an offset *ABABA*... repeat pattern, involving no π–π stacking, but Br···aryl interactions.

Comment

There has been a surge of research activity in the development of specific structure architectures involving the self-assembly of molecules or ions into well defined supramolecular arrays. Non-covalent interactions play an important role in organizing structural units in both natural and artificial systems (Desiraju, 1997). In the present work, we report the crystal structure of the title complex, (I), along with some interesting motifs of supramolecularity represented by N—H···Br and C—H···Br hydrogen bonding along with Br···aryl interactions.



(I)

The asymmetric unit of (I) is shown in Fig. 1, and consists of one 2,3-dimethylquinoxalinium cation (henceforth $DmqxH_2$) and two Br^- anions. They all lie on a crystallographic mirror plane, enabling the formation of hydrogen-bonded layers. Bond lengths and angles in the cation are similar to those reported previously (Willett & Twamley, 2001).

The two Br^- anions hydrogen-bond to the NH group of the same cation, thus forming a trimeric unit, which is parallel to (010). Adjacent layers are separated by half the b-axis length (Fig. 2). Details of the hydrogen bonding are given in Table 1. Atom Br1 accepts hydrogen bonds from the NH and HC groups of $DmqxH_2$, while atom Br2 accepts hydrogen bonds from only the NH groups. Both NH groups in (I) act as simple donors to the Br^- anions. The stacking sequence of layers is an offset *ABAB*... repeat pattern. There are no π–π stacking interactions, but the Br^- anions lie over the rings of adjacent layers, giving rise to Br···aryl interactions [Br···centroid distance = 3.29 (8) Å]. These interactions extend over adja-

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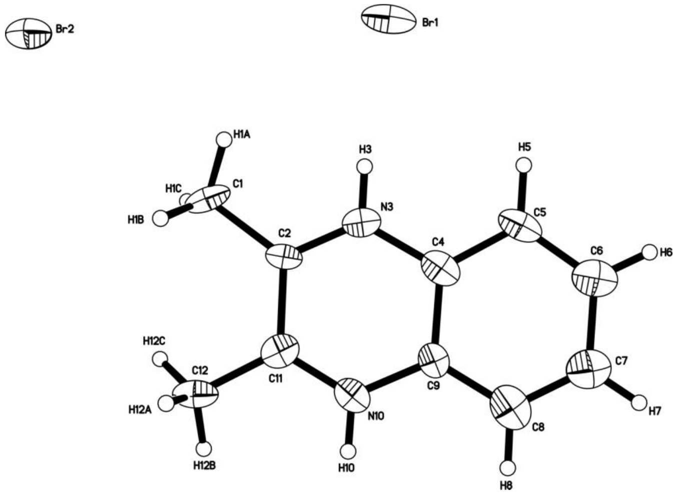

Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

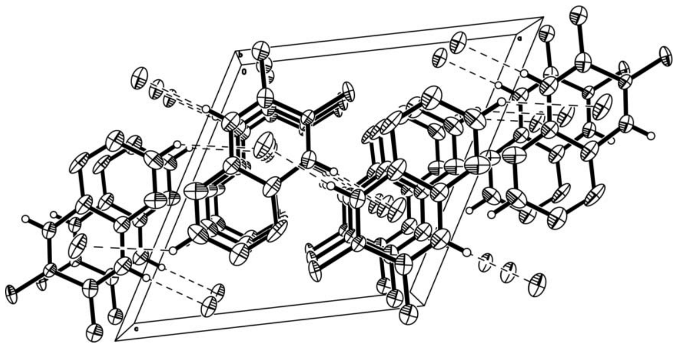

Figure 2
Parallel projection, down the *b* axis, of the crystal packing of compound (I), showing the hydrogen bonding (dashed lines).

cent layers, forming an interlayer aryl···Br···aryl motif, similar to that observed previously (Al-Far & Ali, 2007; Haddad *et al.*, 2006).

Experimental

Small yellow needles of (I) were obtained accidentally from an attempted crystallization of an organic–inorganic hybrid. To a hot absolute ethanol solution (10 ml) of 2,3-dimethylquinoxaline (1 mmol) was added 1 mmol of $CoCl_2$ dissolved in 10 ml of absolute ethanol. The mixture was then treated with 60% HBr and Br_2 (2–3 ml each), stirred and heated for 2 h. The solution was then allowed to cool slowly to room temperature. Crystals appeared after approximately 48 h.

Crystal data

$C_{10}H_{12}N_2^{2+}\cdot 2Br^-$
$M_r = 320.02$
Monoclinic, $P2_1/m$
$a = 9.920$ (4) Å
$b = 6.582$ (3) Å
$c = 9.998$ (4) Å
$\beta = 118.929$ (6)°
$V = 571.4$ (4) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 7.06$ mm^{-1}
$T = 297$ (2) K
0.34 × 0.13 × 0.09 mm

Data collection

Bruker/Siemens SMART APEX diffractometer
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2002)
$T_{\min} = 0.184$, $T_{\max} = 0.529$
1576 measured reflections
1126 independent reflections
1126 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.191$
$S = 1.13$
1560 reflections
86 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 2.28$ e Å^{-3}
$\Delta\rho_{\min} = -1.06$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···Br1	0.86	2.28	3.135 (9)	175
N10—H10···Br2$^{\rm i}$	0.86	2.27	3.126 (10)	178
C7—H7···Br1$^{\rm i}$	0.93	2.95	3.731 (15)	142

Symmetry code: (i) $x - 1, y, z$.

The data were rotationally twinned and were deconvoluted giving a two-component twin relationship: 179.8° rotation about the reciprocal axis 1.000, 0.000, 0.002, with a refined twinning ratio of 0.347 (3). The matrix used to relate the second orientation to the first domain is: 0.998/−0.004/0.962, 0.000/−1.000/−0.002, 0.004/0.004/−0.998. Each cell component was refined on all observed reflections. The methyl substituents are disordered about the mirror plane; the H atoms have occupancies of 0.5. All H atoms were initially located in a difference Fourier map and were subsequently refined using a riding model, with C—H distances of 0.98 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H atoms; C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for quinoxaline-ring H atoms, and N—H = 0.86 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm N})$ for the protonated quinoxaline. The methyl groups were allowed to rotate freely about their local threefold axes. The highest and lowest peaks in the final difference Fourier synthesis are 1.08 Å from atom Br1 and 1.24 Å from atom Br2, respectively.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2004); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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