trans-Cyclohexane-1,4-diammonium dibromide

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.049
wR factor = 0.113
Data-to-parameter ratio = 35.8

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

A structure consisting of alternating organic and inorganic
layers is exhibited by the title compound, $C_6H_{16}N_2^{2+}\cdot2Br^-$.
The ammonium groups and bromide anions interact via
hydrogen bonds to form a two-dimensional hydrogen-bond
network.

Comment

The crystal structure of (I) was determined as part of an
ongoing investigation of the structural characteristics and non-
covalent interactions of organic–inorganic hybrid salts. The
structure of the corresponding chloride salt, trans-1,4-
diaminocyclohexane dihydrochloride, (II), has been reported
(Dunitz & Strickler, 1966), but the chloride and bromide salts
are not isostructural.
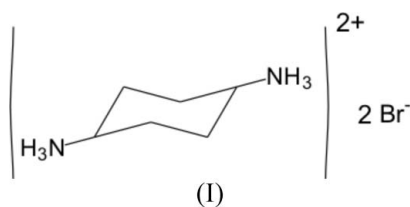
The asymmetric unit of (I) consists of half a trans-1,4-
diammoniocyclohexane cation and one bromide anion; the
cation lies on an inversion centre. Fig. 1 illustrates the mol-
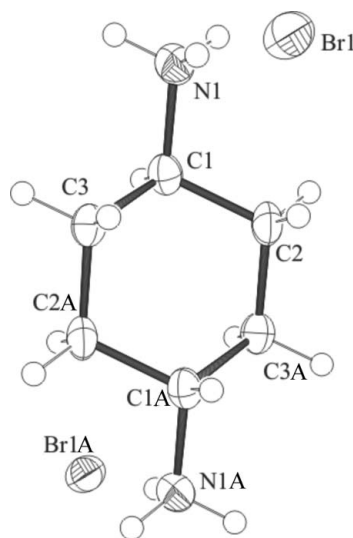ecular geometry and atomic labelling scheme.

Figure 1
The molecular structure of (I) showing the atomic numbering scheme and
displacement ellipsoids at the 50% probability level [symmetry operator:
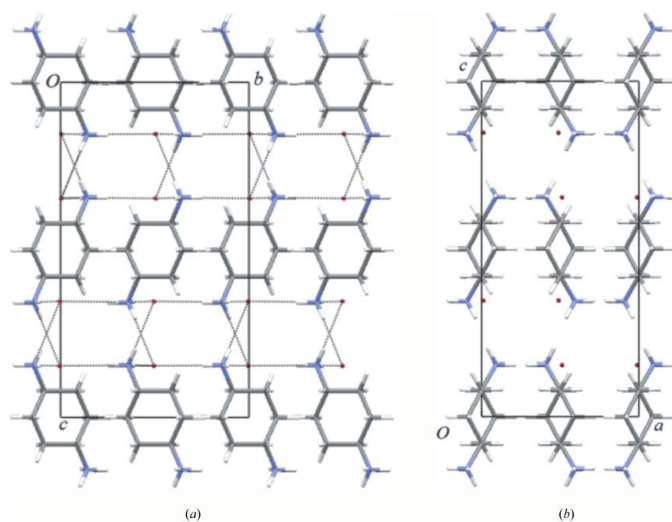(A) $-x$, $-y$, $-z$] (ORTEP-3; Farrugia, 1997).

Figure 2
(*a*) Packing diagram for (I), viewed down the *a* axis. Hydrogen bonding interactions are shown as dotted lines. (*b*) View down the *b* axis. (*Mercury*; Macrae *et al.*, 2006).
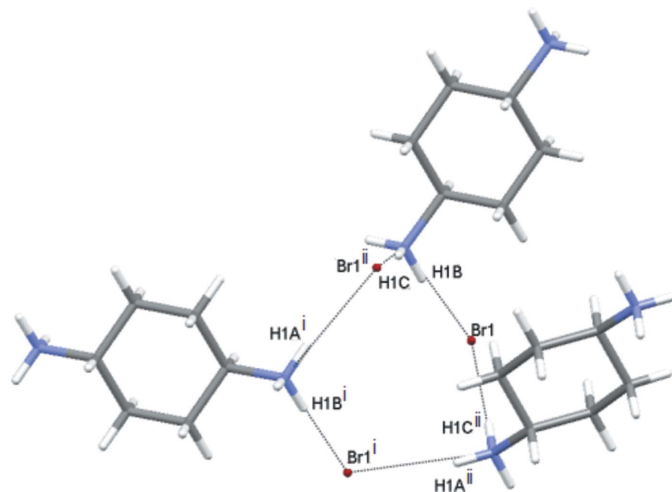

Figure 3
Hydrogen-bonding interactions (*Mercury*; Macrae *et al.*, 2006). [Symmetry codes: (i) $x + \frac{1}{2}$, y, $-z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}$, $y + \frac{1}{2}$, z.]

As illustrated in Fig. 2, the crystal structure is composed of alternating organic and inorganic layers, parallel to the (001) plane of the unit cell. The ammonium groups and bromide anions constitute the inorganic layer, while the cyclohexane rings, which adopt a chair conformation, form the organic layer. Viewed down the *a* axis, cations in neighbouring layers display alternating tilt directions (Fig. 2). However, within a layer, neighbouring tilted cations alternate in orientation (Fig. 3). Interestingly, the structure reported for (II) is, in general, very similar to that of (I); however, the cations in a particular layer all have the same orientation.

In the inorganic layer the ammonium groups and bromide anions interact *via* N^+—$H \cdots Br^-$ charge-assisted hydrogen bonds, with each ammonium group forming three classical hydrogen bonds to three different bromide anions. Each bromide anion, in turn, interacts with three different ammonium groups. A two-dimensional hydrogen-bonding network,

parallel to the *ab* plane, is formed, consisting of hydrogen-bonded rings of the type $R_6^3(9)$ (Fig. 3). Hydrogen-bonding parameters are listed in Table 1.

Experimental

trans-1,4-Diaminocyclohexane dihydrobromide was prepared by the dropwise addition of HBr (48%, Fluka) to a solution of *trans*-1,4-diaminocyclohexane (+99%, Fluka, 0.421 g) in 35 ml of chloroform (99%, Saarchem) at room temperature. The solution was allowed to evaporate at room temperature, and a precipitate formed after four days. The precipitate was filtered and recrystallized from distilled water at room temperature over a period of five weeks, yielding good quality crystals.

Crystal data

$C_6H_{16}N_2^{2+} \cdot 2Br^-$	$Z = 4$
$M_r = 276.03$	$D_x = 1.754$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 7.4264\ (6)$ Å	$\mu = 7.70$ mm^{-1}
$b = 8.9074\ (6)$ Å	$T = 295\ (2)$ K
$c = 15.8018\ (14)$ Å	Block, colourless
$V = 1045.29\ (14)$ Å^3	$0.40 \times 0.30 \times 0.20$ mm

Data collection

Oxford Diffraction Excalibur2 diffractometer	8858 measured reflections
ω scans	1683 independent reflections
Absorption correction: multi-scan (Blessing, 1995)	1118 reflections with $I > 2\sigma(I)$
$T_{min} = 0.074$, $T_{max} = 0.216$	$R_{int} = 0.043$
	$\theta_{max} = 31.9°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 2.6029P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.113$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.08$	$\Delta\rho_{max} = 0.66$ e Å^{-3}
1683 reflections	$\Delta\rho_{min} = -0.76$ e Å^{-3}
47 parameters	Extinction correction: *SHELXL97*
H-atom parameters constrained	Extinction coefficient: 0.049 (2)

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

D—$H \cdots A$	D—H	$H \cdots A$	$D \cdots A$	D—$H \cdots A$
N1—H1$A \cdots$Br1^i	0.89	2.46	3.308 (3)	159
N1—H1$B \cdots$Br1^{ii}	0.89	2.45	3.317 (3)	166
N1—H1$C \cdots$Br1^{iii}	0.89	2.46	3.343 (3)	173

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

All H atoms were placed in calculated positions, with methylene C—H distances of 0.97 Å, a methine C—H distance of 0.98 Å, and N—H distances of 0.89 Å, and were refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(N)$ of the parent atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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