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Butane-1,4-diammonium dibromide

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The crystal structure of butane-1,4-diammonium dibromide, $C_4H_{14}N_2^{2+}\cdot 2Br^-$, exhibits ionic–inorganic layers separated by organic hydrocarbon layers. The organic hydrocarbon layers pack in a stacked herring-bone manner with hydrogen bonds to the bromide ions. The cation sits on a centre of inversion. The structure is compared with that of butane-1,4-diammonium dichloride and butane-1,4-diammonium diiodide.

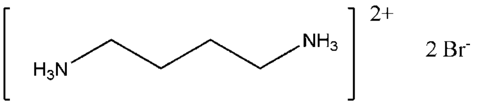
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.045
wR factor = 0.131
Data-to-parameter ratio = 28.5

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

Comment

As part of an ongoing study of the structural characteristics of organic–inorganic layered diammonium salts, the crystal structure of butane-1,4-diammonium dibromide, (I), was determined. A search of the Cambridge Structural Database (Version 5.27, November 2005 release; Allen, 2002) revealed that the crystal structure of butane-1,4-diammonium dichloride was redetermined and published 26 years ago (Chandrasekhar & Pattabhi, 1980). Recently, the crystal structure of butane-1,4-diammonium diiodide was studied and published (Lemmerer & Billing, 2006). The present study completes the series of halide salts and shows all three compounds to be isostructural. The dichloride structure was shown to exhibit a short N···Cl non-bonded contact that links the two-dimensional layers along the *a* direction. Butane-1,4-diammonium dibromide exhibits the same interaction.



(I)

The butane-1,4-diammonium cation sits on a centre of inversion and therefore the asymmetric unit contains one anion and half of the cation (Fig. 1).

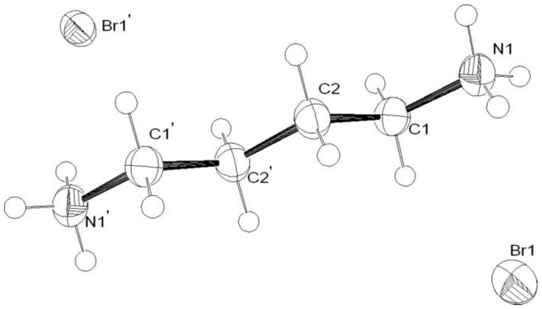


Figure 1
Molecular structure of (I), with the atomic numbering scheme and displacement ellipsoids drawn at the 50% probability level. Atoms labelled with ' are at the symmetry position (1 − x, 1 − y, 1 − z).

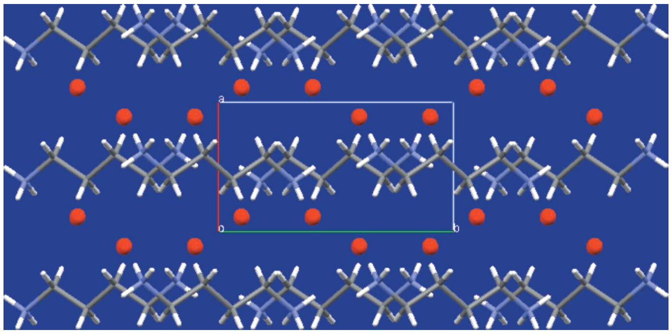


Figure 2
Packing diagram of (I), viewed down the *c* axis. Each layer of butane-1,4-diammonium cations is sandwiched by layers of bromide ions.

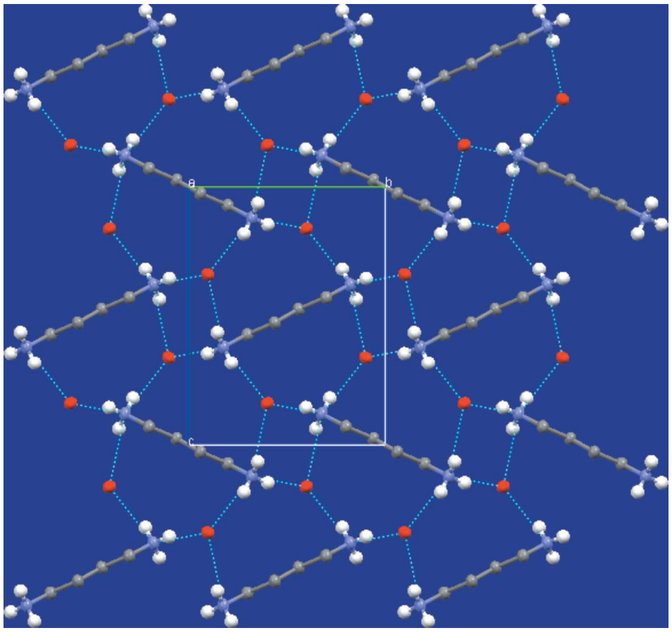


Figure 3
The two-dimensional hydrogen-bonded (dotted lines) network in (I), viewed down the *a* axis.

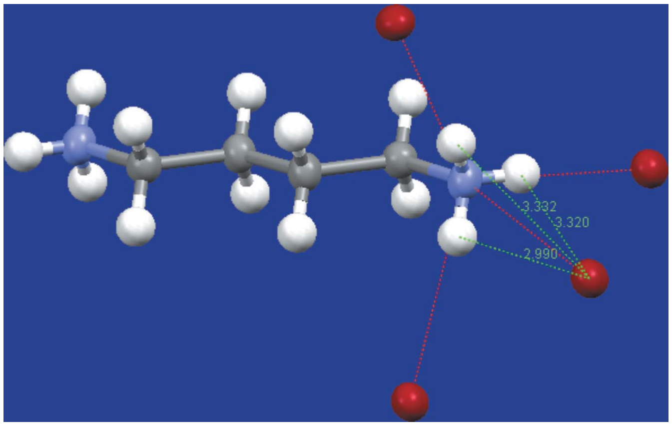


Figure 4
A view of (I), showing the fourth short contact with particular focus on the hydrogen bonding of the three ammonium H atoms with the Br^- anion.

Fig. 2 illustrates the packing of the compound viewed down the *c* axis. The packing arrangement shown is one-dimensional, with a single layer of butane-1,4-diammonium cations sandwiched between two layers of bromide anions, thus forming an alternating organic–inorganic structure. The butane-1,4-diammonium cations pack in a herring-bone manner (Fig. 3).

Fig. 4 clearly shows the occurrence of four short N···Br non-bonded contacts. Three of these contacts may be ascribed to charge-assisted hydrogen-bond formation and the fourth is a short contact directed approximately along the extension of the C—N bond. This fourth contact may be viewed as also involving H atoms since the Br^- anion is at similar distances from the three atoms H1*C*, H1*D* and H1*E* (Table 1).

The N—H···Br hydrogen bonds (Table 1) form an extensive network. Two ammonium H atoms, H1*C* and H1*D*, form hydrogen-bonded rings with graph-set notation $R^2_2(8)$ while hydrogen-bonded rings with graph-set notation $R^2_3(13)$ involve all three ammonium H atoms. The smaller ring is rectangular in shape, with both the short and the long edges of the rectangle sharing sides with the larger ring. The larger ring has five sides, of which one is the butane-1,4-diammonium cation. All the edges of the rings are shared, forming an infinite network in the *ac* plane.

Experimental

The title compound was prepared by adding 1,4-diaminobutane (0.050 g, 0.567 mmol) to 47% hydrobromic acid (2 ml, 37 mmol) in a sample vial. The mixture was then refluxed at 363 K for 2 h. The solution was cooled slowly at 2 K h^{-1} to room temperature. Colourless crystals of butane-1,4-diammonium dibromide were collected.

Crystal data

$C_4H_{14}N_2^{2+}\cdot 2Br^-$
$M_r = 249.99$
Monoclinic, $P2_1/c$
$a = 4.7107$ (9) Å
$b = 8.5491$ (15) Å
$c = 11.229$ (2) Å
$\beta = 93.037$ (4)°
$V = 451.57$ (14) Å^3
$Z = 2$
$D_x = 1.839$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 8.90$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.44 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.056$, $T_{max} = 0.190$ (expected range = 0.024–0.083)
2321 measured reflections
1113 independent reflections
942 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.131$
$S = 0.99$
1113 reflections
39 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0984P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.50$ e Å^{-3}
$\Delta\rho_{min} = -1.64$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.45 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···Br1^{i}	0.89	2.50	3.355 (4)	161
N1—H1D···Br1	0.89	2.62	3.425 (4)	150
N1—H1E···Br1^{ii}	0.89	2.54	3.404 (4)	164
N1—H1C···Br1^{iii}	0.89	3.32	3.393 (3)	87
N1—H1D···Br1^{iii}	0.89	2.99	3.393 (3)	110
N1—H1E···Br1^{iii}	0.89	3.33	3.393 (3)	86

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

H atoms were geometrically positioned and refined in the riding-model approximation, with C—H = 0.97 Å, N—H = 0.89 Å, and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(N). The highest peak in the final difference map is 0.82 Å from Br1 and the deepest hole is 0.90 Å from Br1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; 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: *WinGX* (Farrugia, 1999), *PLATON* (Spek, 2003) and *publCIF* (Westrip, 2006).

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