Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Phenylethylammonium bromide

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Received 7 November 2006
Accepted 28 November 2006

Key indicators

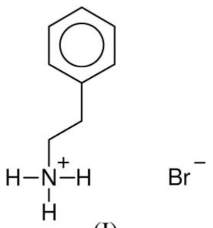
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.032
wR factor = 0.059
Data-to-parameter ratio = 32.5

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

2-Phenylethylammonium bromide, $C_8H_{12}N^+\cdot Br^-$, adopts a layered structure consisting of alternating hydrophilic and hydrophobic regions. The ammonium groups and bromide anions interact through $N^+—H\cdots Br^-$ hydrogen bonds, forming *transoid* one-dimensional ladders, which are further linked by electrostatic $N^+\cdots Br^-$ interactions into two-dimensional sheets.

Comment

The crystal structure of 2-phenylethylammonium bromide, (I) (Fig. 1), was determined as part of an ongoing study of the structural characteristics and hydrogen-bonding interactions of organic salts consisting of arylammonium cations and halide anions. The unit-cell parameters of (I) have been reported previously by Tsoucaris (1961), but fractional coordinates were not given in that report. The crystal structure of the analogous chloride salt has also been described previously (Tsoucaris, 1961; Horn *et al.*, 1990), and (I) is isostructural to it. Compared to the unit-cell parameters of the chloride salt [a = 4.603 (1) Å, b = 5.906 (1) Å, c = 32.360 (1) Å; Horn *et al.*, 1990], the b parameter in (I) is slightly elongated and the c parameter is slightly shortened. As expected, the unit-cell volume of (I) is larger than that of the chloride salt [880 (1) Å^3].



(I)

The crystal structure of (I) consists of layers lying parallel to the *ab* plane, with alternating hydrophobic regions (containing the ammonium groups and bromide anions) and hydrophilic regions (containing the rest of the organic cations) (Fig. 2). In the organic cation, the ethylammonium chain is close to a fully extended all-*trans* conformation, with the N1—C1—C2—C3 torsion angle equal to 173.6 (2)°. The benzene rings pack in a non-interdigitated fashion, with the ring plane forming a dihedral angle of 55.68 (7)° to the *ab* plane. In this region, the shortest centroid-to-centroid distance between benzene rings is 5.590 (2) Å.

In the hydrophilic regions, ammonium groups and bromide anions interact *via* $N^+—H\cdots Br^-$ hydrogen bonds (Table 1). Each H atom of the ammonium group forms three short,

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doi:10.1107/S1600536806051488

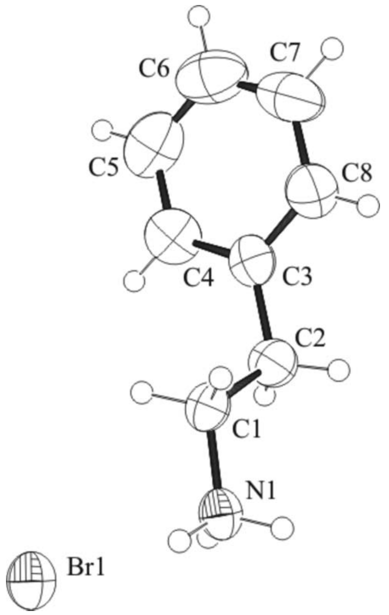

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms.

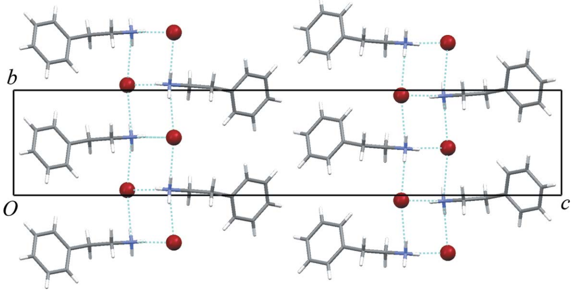

Figure 2
View of (I) down the *a* axis, showing layers lying parallel to the *ab* plane and $N^+—H\cdots Br^-$ hydrogen bonds (blue dotted lines) forming extended one-dimensional ladders.

charge-assisted hydrogen bonds to three different bromide anions, with $N^+\cdots Br^-$ distances ranging from 3.3186 (19) Å to 3.370 (2) Å. These interactions define a *transoid* one-dimensional hydrogen-bonded ladder (Fig. 2). A fourth, longer $N^+\cdots Br^-$ contact [$N1\cdots Br1^i$ = 3.459 (2) Å; symmetry code: (i) $-1 + x, y, z$] links these hydrogen-bonded ladders into corrugated two-dimensional sheets (Fig. 3). A similar sheet structure has been reported for ethylammonium bromide (Jellinek, 1958; Bond, 2005). In both that structure and (I), adjacent sheets are stacked in a parallel offset fashion, with $Br^-\cdots N^+\cdots Br^-$ angles close to 90°.

Experimental

2-Phenylethylammonium bromide was synthesized by dropwise addition of HBr (8.2 ml, 72.9 mmol, 48%, Fluka) to a solution of 2-phenylethylamine (5.3 ml, 42.2 mmol, Aldrich, 99%) in chloroform (30 ml). The resulting precipitate was filtered off. The crystal used for this structure determination was crystallized from an aqueous solution of 2-phenylethylammonium bromide (0.500 g, 2.47 mmol) and $CoBr_2$ (Aldrich, 99%, 0.271 g, 1.24 mmol) (2:1 molar ratio), open to the atmosphere, at room temperature over a period of eight weeks.

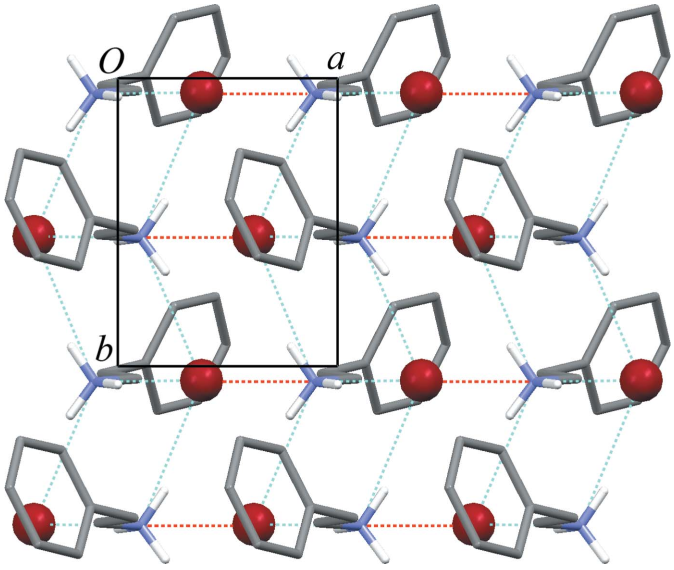

Figure 3
View of (I) down the *c* axis, showing a single two-dimensional sheet in the *ab* plane. $N^+—H\cdots Br^-$ hydrogen bonds are shown as blue dotted lines, and the longer $N^+\cdots Br^-$ contacts between ladders are shown as red dotted lines. H atoms bound to C atoms are omitted.

Crystal data

$C_8H_{12}N^+\cdot Br^-$
M_r = 202.10
Orthorhombic, $P2_12_12_1$
a = 4.6871 (4) Å
b = 6.1419 (4) Å
c = 32.047 (2) Å
V = 922.56 (12) Å^3
Z = 4
D_x = 1.455 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 4.39 mm^{-1}
T = 295 (2) K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Oxford Diffraction Excalibur2 CCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.340, T_{max} = 0.419
9448 measured reflections
2958 independent reflections
2063 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 32.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.059
S = 1.06
2958 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}
Absolute structure: Flack (1983), 1047 Friedel pairs
Flack parameter: 0.029 (15)

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
$N1—H1A\cdots Br1$	0.89	2.49	3.360 (2)	166
$N1—H1B\cdots Br1^i$	0.89	2.46	3.3186 (19)	162
$N1—H1C\cdots Br1^{ii}$	0.89	2.51	3.370 (2)	163

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

H atoms were placed in calculated positions, with methylene C—H = 0.97 Å, aromatic C—H = 0.93 Å, and N—H = 0.89 Å, and were refined using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(N).

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* (Bruno *et al.*, 2002); software used to prepare material for publication: *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

This work was funded by the University of KwaZulu-Natal Research Office, and the National Research Foundation (GUN:2054350).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Bond, A. D. (2005). *Cryst. Growth Des.* **5**, 755–771.

Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Horn, E., Tiekink, E. R. T., Jones, G. P., Naiola, B. P. & Paleg, L. G. (1990). *Acta Cryst.* C**46**, 1575–1576.

Jellinek, F. (1958). *Acta Cryst.* **11**, 626–631.

Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171.29.9. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Tsoucaris, G. (1961). *Acta Cryst.* **14**, 909–914.