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(*R*)-1-Phenylethanaminium bromide

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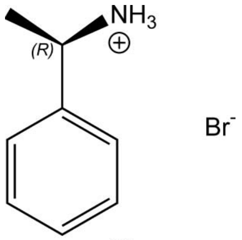
The title compound, $C_8H_{12}N^+\cdot Br^-$, was obtained from an aqueous solution of (*R*)-1-phenylethanamine and racemic 2,3-dibromosuccinic acid. It features a three-dimensional network of N—H···Br hydrogen bonds.

Key indicators
Single-crystal X-ray study
T = 297 K
Mean *σ*(C–C) = 0.008 Å
R factor = 0.049
wR factor = 0.081
Data-to-parameter ratio = 22.8

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

Comment

We are currently studying the crystal chemistry of 2,3-dibromosuccinic acids and their salts and recently reported the crystal structure of (2*R*,3*S*)-dibromosuccinic acid (Eriksson *et al.*, 2006). An attempt to crystallize the phenylethanaminium salt of (*R*,*R*)-dibromosuccinic acid yielded the compound (*R*)-1-phenylethanaminium–(*S*,*S*)-2,3-dibromosuccinate–(*R*,*R*)-2,3-dibromosuccinic acid–water (2/1/1/2) (Fischer, 2006). This compound had been obtained from half an equivalent of the amine and racemic 2,3-dibromosuccinic acid in aqueous solution. The reaction of the acid with an equimolar amount of the amine yielded a yellow amorphous precipitate. From the remaining solution, crystals of the title compound were obtained upon evaporation at 323 K.



(I)

The structure features (*R*)-1-phenylethanaminium cations, whose geometry is unexceptional, and bromide anions (Fig. 1). The most prominent feature in the crystal structure is the hydrogen-bonding pattern (Fig. 2 and Table 1). Each NH hydrogen acts a hydrogen-bond donor. Hence, three hydrogen bonds are formed between N and three different bromide ions; each bromide ion functions in turn as an acceptor for three hydrogen bonds, yielding a layered network parallel to the *ab* plane (Fig. 2).

Experimental

Racemic 2,3-dibromosuccinic acid was prepared as described by Fischer (2006). The acid (282 mg) was mixed with the (*R*)-phenylethanamine [0.26 (1) ml, Fluka, purum] in demineralized water (5 ml). The solution was heated to 323 K. Almost immediately, precipitation occurred and this was filtered off. (In an examination with X-ray powder diffractometry, it turned out to be amorphous. Attempts to obtain single crystals from this yellow phase have so far been unsuccessful.) The remaining solution was left on the heating plate at 323 K. Within a day, single crystals of the title compound were obtained.

Crystal data

$C_8H_{12}N^+ \cdot Br^-$
$M_r = 202.10$
Orthorhombic, $P2_12_12_1$
$a = 5.5319\ (9)$ Å
$b = 8.6962\ (14)$ Å
$c = 19.364\ (4)$ Å
$V = 931.5\ (3)$ Å^3
$Z = 4$
$D_x = 1.441$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.35$ mm^{-1}
$T = 297$ K
Needle, colourless
0.16 × 0.04 × 0.03 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
ω scans
Absorption correction: none
17585 measured reflections
2122 independent reflections
1500 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.116$
$\theta_{\rm max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.081$
$S = 1.16$
2122 reflections
93 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0116P)^2 + 0.763P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.49$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.35$ e Å^{-3}
Absolute structure: Flack (1983), 845 Friedel pairs
Flack parameter: 0.01 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Br1$^{\rm i}$	0.89	2.51	3.379 (4)	166
N1—H1B···Br1$^{\rm ii}$	0.89	2.40	3.268 (4)	164
N1—H1C···Br1$^{\rm iii}$	0.89	2.46	3.347 (4)	173

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

H atoms were placed at calculated positions and refined using a riding model with C—H = 0.93 Å, $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for aromatic, C—H = 0.98 Å, $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for CH, C—H = 0.96 Å, $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for CH$_3$, and N—H = 0.89 Å, $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm N})$ for NH.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX*/*LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *MAXUS* (Mackay *et al.*, 1999).

The Swedish Research Council (VR) is acknowledged for providing funding for the single-crystal diffractometer.

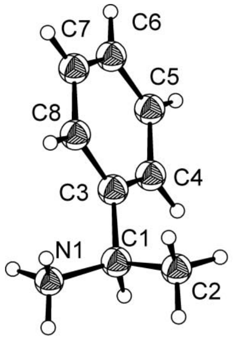


Figure 1
The asymmetric unit of (*R*)-1-phenylethanaminium bromide. Displacement ellipsoids are drawn at the 50% probability level.

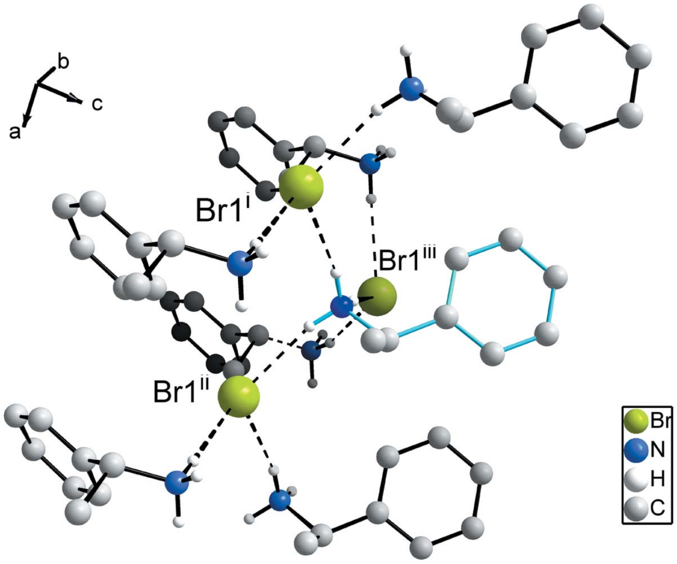


Figure 2
The hydrogen-bonding network in the title compound. Hydrogen bonds are dashed. The cation in the asymmetric unit is indicated by blue bonds. All C-bound H atoms have been omitted.

References

Brandenburg, K. (2006). *DIAMOND*. Release 3.1b. Crystal Impact GbR, Bonn, Germany.

Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.

Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.

Eriksson, M., Fischer, A., Lind, J. & Zazzi, Å. (2006). *Acta Cryst.* E**62**, o200–o201.

Fischer, A. (2006). *Acta Cryst.* E**62**, o1281–o1283.

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

Mackay, S., Gilmore, C. J., Edwards, C., Stewart, N. & Shankland, K. (1999). *MAXUS*. Bruker–Nonius, The Netherlands, MacScience, Japan, and The University of Glasgow, Scotland.

Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.

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