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Trimethylammonium bromide at 100 K

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The title compound, $C_3H_{10}N^+{\cdot}Br^-$, is composed of hydrogen-bonded $(CH_3)_3NH^+$ and Br^- ions. The N, Br and CH of one methyl substituent lie on a mirror plane that relates the two remaining CH_3 groups by symmetry.

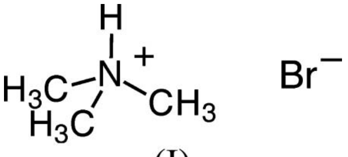
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(N–C) = 0.006 Å
R factor = 0.048
wR factor = 0.050
Data-to-parameter ratio = 17.3

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

Comment

The unit-cell dimensions of trimethylammonium bromide, (I), at room temperature (283–303 K) were determined from powder diffraction data by Mussgnug (1941). The compound readily forms from trimethylamine and HBr, for instance, as a by-product in bromine trimethylamine exchange reactions (Hartung *et al.*, 2006). Colourless needles that separated from a solution of (I) in CH_2Cl_2–petroleum ether were investigated by X-ray diffraction at 100 K in order to document its hitherto unknown solid-state geometry.


(I)

Trimethylammonium bromide, (I), crystallizes in $P2_1/m$ (Z = 2). The space group and unit-cell dimensions agree with the values determined by Mussgnug (1941) [$P2_1/m$, a = 6.86 Å, b = 8.16 Å, c = 5.41 Å, β = 107.5°, D_x = 1.587 g cm^{-3}]. A 3% decrease of the unit-cell volume from the powder cell is in the expected range for data collected at 100 K as opposed to the room-temperature powder data. The N atom is positioned in the centre of a flattened tetrahedron, which is formed by the three methyl C atoms and H1*D* (Fig. 1, Table 1). A mirror plane that runs through N, Br, C1 and H1*C* relates C2 to C2a [symmetry code: (a) $x, -y + \frac{1}{2}, z$; Fig. 1]. The C—N distances and C—N–C angles in (I) agree with values reported for trimethylammonium chloride (Lindgren & Olovsson, 1968), trimethylammonium iodide (Sheldrick & Sheldrick, 1970) and gaseous trimethylamine [electron diffraction: C—N = 1.47 (2) Å and C—N—C = 108 (4)°; Brockway & Jenkins, 1936].

In the unit cell, $(CH_3)_3NH^+$ and Br^- ions are linked *via* hydrogen-bonding interactions [N1···Br1 = 3.262 (7) Å and N1—H1*D*···Br1 = 165 (2)°; Fig. 2], thus leading to coordination numbers of 1 for Br and 4 for N. The packing of $(CH_3)_3NHBr$ occurs in infinite columns of Br^- ions and trimethylammonium cations (Fig. 3). In spite of the fact that the atomic parameters of the ammonium ions and the associated hydrogen-bonding geometries are similar, packing of

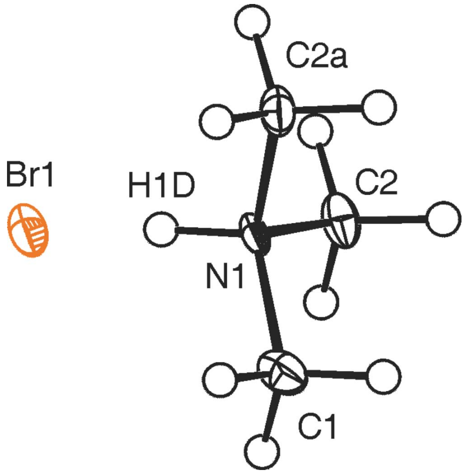


Figure 1
The molecular structure of (I) in the solid state. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (*a*) $x, \frac{1}{2} - y, z$.]

the three thus far investigated trimethylammonium halides $(CH_3)_3NHX$ (X = Cl, Br or I; space group $P2_1/m$) leads to different unit-cell dimensions, which is caused by a gradual increase of the N$\cdots X$ distance along the series N$\cdots$Cl [3.005 (5) Å] < N$\cdots$Br [3.262 (7) Å] < N$\cdots$I [3.46 (4) Å] (Lindgren & Olovsson, 1968; Sheldrick & Sheldrick, 1970).

Experimental

Crystals suitable for X-ray diffraction were obtained by slowly concentrating a solution of (I) in CH_2Cl_2–petroleum ether (1:2 *v*/*v*) at 298 K.

Crystal data

$C_3H_{10}N^+\cdot Br^-$
M_r = 140.03
Monoclinic, $P2_1/m$
a = 5.349 (3) Å
b = 8.023 (4) Å
c = 6.790 (3) Å
β = 105.70 (4)°
V = 280.5 (2) Å^3
Z = 2
D_x = 1.658 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 407 reflections
θ = 3.1–21.2°
μ = 7.17 mm^{-1}
T = 100 (2) K
Needle, colourless
0.10 × 0.04 × 0.02 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
ω and φ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2002)
T_{min} = 0.534, T_{max} = 0.870
2059 measured reflections
606 independent reflections
449 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 26.4°
$h = -6 \rightarrow 5$
$k = -9 \rightarrow 10$
$l = -6 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.050
S = 0.89
606 reflections
35 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0093P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

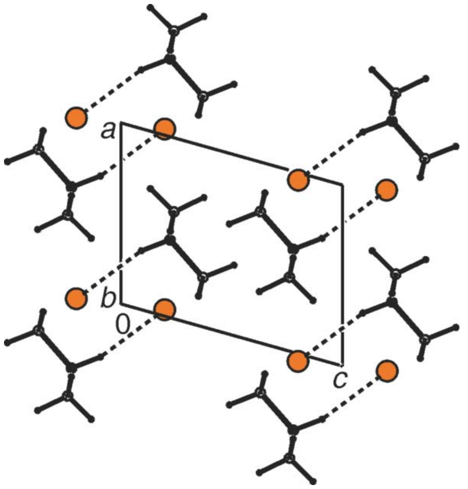


Figure 2
The hydrogen bonding (dashed lines) in (I), viewed along [010]. Br^- ions are depicted in orange.

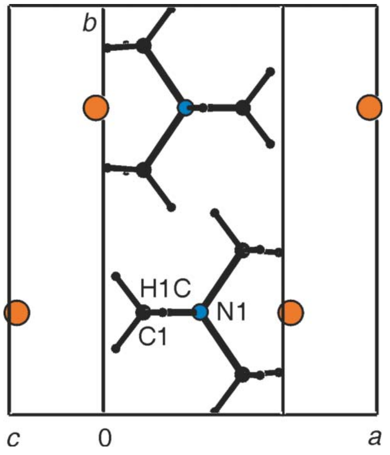


Figure 3
The packing of (I) in the unit cell, showing the mirror plane that runs through N (blue), Br (orange), C1 and H1*C*, as viewed along [001].

Table 1
Selected bond lengths (Å).

C1—N1	1.487 (8)	C2—N1	1.474 (4)

Atoms H1*A*, H1*C*, H1*D* were located in a difference Fourier map and their atomic coordinates were refined, with U_{iso}(H) set to 1.2U_{eq} of the parent atom. All other H atoms were positioned geometrically and treated as riding atoms, with C—H = 0.98 Å and with U_{iso}(H) set to 1.2U_{eq}(C). The maximum electron-density peak is located approximately 1.1 Å from atom Br1.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON2002* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997, 2005); software used to prepare material for publication: *SHELXL97*.

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o572 Hartung *et al.* • $C_3H_{10}N^+\cdot Br^-$ *Acta Cryst.* (2006). E**62**, o570–o572