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N-*n*-Butylpyridinium bromide

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The title compound, $C_9H_{14}N^+\cdot Br^-$, was synthesized by the reaction of pyridine and *n*-butyl bromide. The crystal packing is stabilized by intermolecular C—H···Br hydrogen bonds.

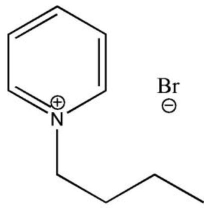
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.020 Å
Disorder in main residue
R factor = 0.047
wR factor = 0.138
Data-to-parameter ratio = 8.4

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

Comment

Pyridinium halides and their binary mixures with metal halides can be utilized to study the effects of varying the Lewis acid-base character (Osteryoung *et al.*, 1978), investigating complex ion formation (Angell *et al.*, 1976), and further characterizing the supercooled region of the liquid state (Easteal *et al.*, 1970). The crystal structure of *N*-*n*-butylpyridinium chloride has been reported (Ward *et al.*, 1986). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The *n*-butyl chain is disordered over two orientations, and both disordered components are in the extended configuration with torsion angles C1—C2—C3—C4 of 168 (2)° and C1′-C2′-C3′-C4 of

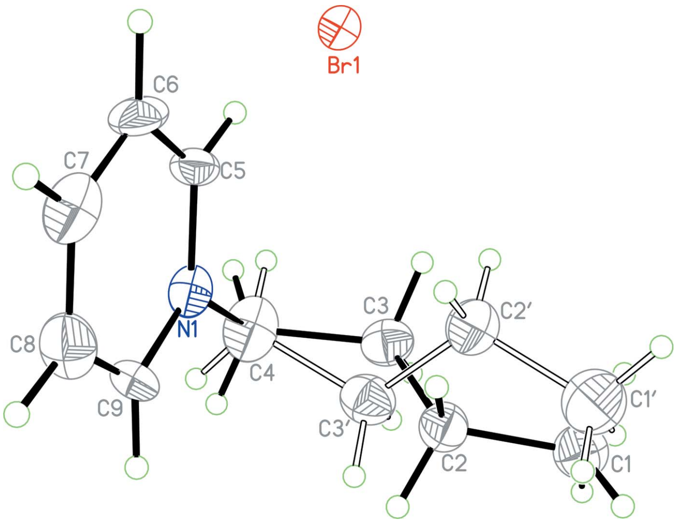


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Both disordered components of the *n*-butyl chain are shown.

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172 (3)°. The orientation of the *n*-butyl substituent with respect to the pyridinium ring is described by the torsion angles C9—N1—C4—C3 of −97.5 (19)° and C9—N1—C4—C3′ of −70 (2)°. In the crystal structure, molecules are linked by C—H···Br hydrogen bonds (Table 1), forming a three-dimensional network (Fig. 2).

Experimental

N-butyl bromide (32.40 ml) was added to 50 ml anhydrous cyclohexane solution of pyridine (48.53 ml) at 333 K. After stirring for 24 h, two layers were formed. The top layer containing the unreacted starting materials was decanted. The bottom layer, a yellow solid phase, was separated into two parts. One part was recrystallized by the addition of acetone to form white crystals while the other part was dissolved in dried acetonitrile. Crystals of compound (I) were obtained by using the white crystals as seed crystals in the latter mixed solution and allowing the mixture to stand overnight. Each starting material was distilled in advance under reduced pressure with 3A molecular sieve (WAKO) and all operations were carried out under a nitrogen atmosphere.

Crystal data

$C_9H_{14}N^+\cdot Br^-$
$M_r = 216.12$
Orthorhombic, $P2_12_12_1$
$a = 8.3040$ (17) Å
$b = 10.783$ (2) Å
$c = 11.699$ (2) Å
$V = 1047.6$ (3) Å^3
$Z = 4$
$D_x = 1.370$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10$–13°
$\mu = 3.87$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.276$, $T_{\max} = 0.461$
1072 measured reflections
1072 independent reflections
641 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 24.9°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 13$
3 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.138$
$S = 0.95$
1072 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.51$ e Å^{-3}
Absolute structure: Flack (1983); 0 Friedel pairs
Flack parameter: −0.02 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4D···Br1^{i}	0.96	2.88	3.778 (16)	155
C6—H6···Br1^{ii}	0.93	2.87	3.743 (13)	156
C8—H8···Br1^{iii}	0.93	2.79	3.715 (16)	172
C9—H9···Br1^{iv}	0.93	2.71	3.618 (12)	166

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

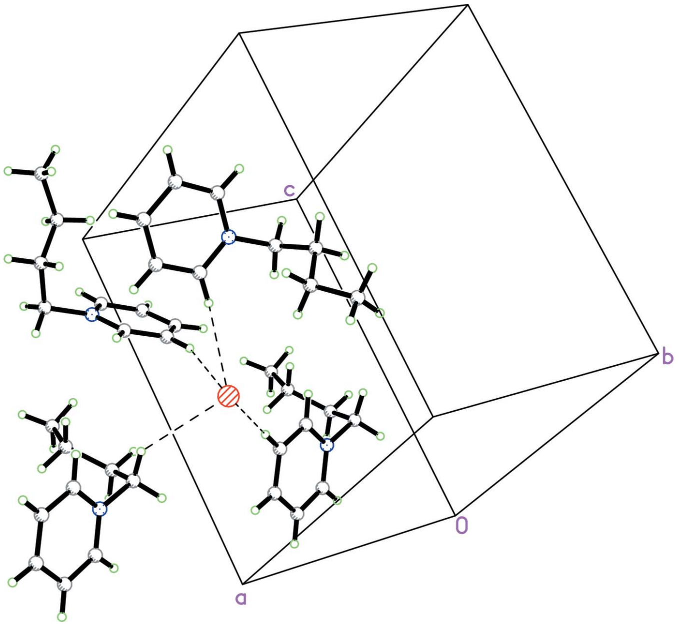

Figure 2
The crystal structure of (I). Dashed lines indicate intermolecular C—H···Br hydrogen bonds.

The *n*-butyl chain was found to be disordered over two orientations. The occupancy factors for the disordered atoms C1/C1′, C2/C2′ and C3/C3′ were initially refined to 0.49 (3)/0.51 (3) and later fixed at 0.50/0.50. The C—C bond lengths involving the disordered atoms were restrained to 1.53 (1) Å. The U^{ij} components of the disordered atoms were approximated to isotropic behaviour. H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å and $U_{\rm iso}$(H) = 1.2–1.5$U_{\rm eq}$(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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