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1-Butylquinolinium bromide

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.076
Data-to-parameter ratio = 22.2

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

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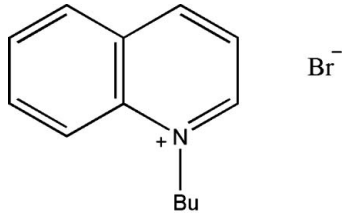
In the title ionic compound, $C_{13}H_{16}N^+\cdot Br^-$, weak C—H···Br hydrogen bonding is the main non-Coulombic interation between cation and anion. Offset face-to-face π–π stacking and C—H···π interactions occur between quinolinium cations.

Comment

Organic molten salts usually show lower melting points and are widely used as phase-transfer catalysts or immobilizing phases for homogeneous catalysts. We report here the crystal structure of the title salt, (I).



(I)

The asymmetric unit is shown in Fig. 1. The torsion angles for the butyl group are given in Table 1. The non-classical C7—H7···Br1 hydrogen bond is the main non-Coulombic interaction between the cation and anion (Table 2). A packing diagram is presented in Fig. 2. The face-to-face separation of 3.41 (4) Å between two offset parallel quinolinium cations indicates the existence of π–π stacking (Steed & Atweed, 2000). The following geometrical data indicate the existence of C—H···π interactions in the crystal structure (Tsuzuki *et al.*, 2000; Desiraju, 2002): *C14—H14A*···*Cg* angle 127°, H14*A*···*Cg* = 3.02 Å and C14···*Cg* = 3.674 (3) Å [*Cg* is the

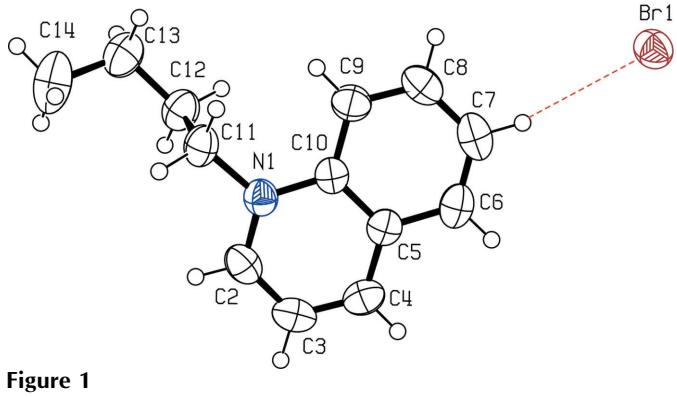


Figure 1
The asymmetric unit of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms). The dashed line indicates the C—H···Br hydrogen bond.

centroid of the C8^{i}-containing ring; symmetry code: (i) $\frac{3}{2} - x$, $-\frac{1}{2} + y$, $\frac{3}{2} - z$]. These weak interactions help to stabilize the crystal structure.

Experimental

The title compound was synthesized by refluxing a mixture of quinoline (30 mmol, 3.84 g) and 1-bromobutane (30 mmol, 5.52 g) in 15 ml 1,4-dioxane in a Schlenk tube for 48 h, and purified by crystallizing from acetonitrile. Single crystals of (I) were obtained by recrystallization from a dichloromethane/diethyl ether solution (1:1) at room temperature.

Crystal data

$C_{13}H_{16}N^{+}\cdot Br^{-}$
M_r = 266.18
Monoclinic, $P2_1/n$
a = 9.8621 (5) Å
b = 11.0998 (6) Å
c = 11.6013 (6) Å
β = 103.002 (1)°
V = 1237.40 (11) Å^3
Z = 4
D_x = 1.429 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.29 mm^{-1}
T = 295 (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.353, T_{max} = 0.518
12191 measured reflections
3061 independent reflections
2488 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.076
S = 1.02
3061 reflections
138 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.5292P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0038 (8)

Table 1
Selected geometric parameters (Å, °).

N1—C11	1.492 (3)	C12—C13	1.520 (3)
C11—C12	1.522 (3)	C13—C14	1.498 (4)
N1—C11—C12—C13	−177.10 (19)	C11—C12—C13—C14	−62.4 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···Br1	0.93	2.97	3.868 (2)	164

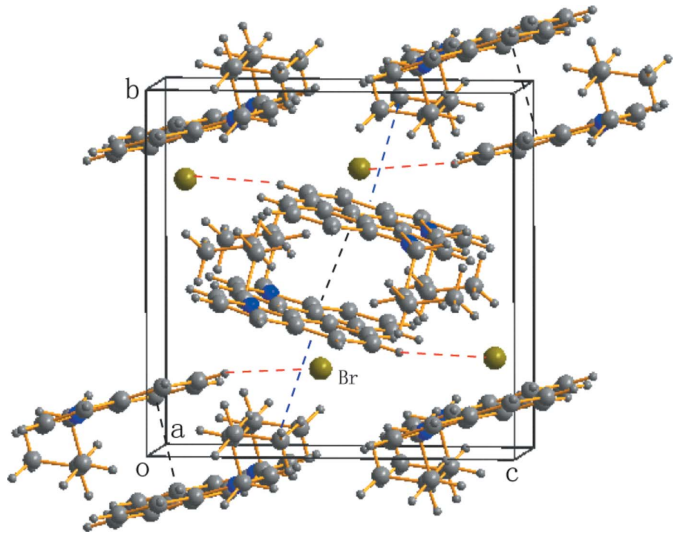


Figure 2
A packing diagram of (I). The C—H···π interactions are indicated by blue dashed lines, offset face-to-face π–π interactions by black dashed lines, and C—H···Br hydrogen bonding by red dashed lines.

H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å. The torsion angle of the methyl group was refined to fit the electron density, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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); software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

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