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6-(3-Iodopropyl)benzo[*f*][1,7]naphthyridin-6-ium iodide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.043
wR factor = 0.095
Data-to-parameter ratio = 21.1

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

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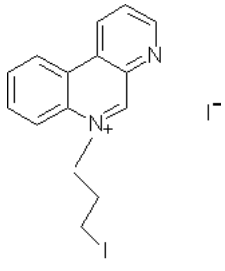
In the title compound, $C_{15}H_{14}IN_2^+\cdot I^-$, the $C_{15}H_{14}IN_2^+$ cations and I^- anions are joined together *via* strong C—H···I hydrogen bonds. In the [010] direction, these cations form positively charged columns, between which the I^- anions are included.

Comment

Much interest has been concentrated in recent years on the synthesis of quaternary aza-aromatic salts due to their potentially high non-linearities (Struganova, 2000; Burtman *et al.*, 2000; Teppner *et al.*, 2000; Andreu *et al.*, 2000; Ashwell *et al.*, 2001; Sitha *et al.*, 2001; Xie *et al.*, 2001) and possible applications in the construction of electronic devices (Gittins *et al.*, 2000; Bryce *et al.*, 2001; Suzuki *et al.*, 2001; Ghaddar *et al.*, 2002). They can also serve as laser dyes (Gawinecki & Trzebiatowska, 2001; Nishigaki & Nakamura, 2001; Isacsson & Westman, 2001; Ashwell *et al.*, 2002; Huang *et al.*, 2002), fluorescent probes (Menger *et al.*, 2001; Camara *et al.*, 2002) and ionic liquids (Aki *et al.*, 2001; Ikeda *et al.*, 2001; Visser *et al.*, 2001), as well as synthons for numerous reactions (Bennasar *et al.*, 2002; Trofimov *et al.*, 2002; Yamada & Morita, 2002) and as biological diagnostic agents (Anastasia *et al.*, 2001; Revesz & Waelchli, 2001). Some show biological, *e.g.* antimicrobial (Beilfuss *et al.*, 2001; Chang *et al.*, 2001; Springer *et al.*, 2001), antidiabetic (Sankaranarayanan, 2001) and anticancer (Saito *et al.*, 2001) activities; they are also promising as nucleic acid intercalators (Juskowiak *et al.*, 2002; Reha *et al.*, 2002). This is the fourth paper of a series concerning benzonaphthyridinium quaternary salts (Marciniak *et al.*, 2002*a*,*b*; Marciniak *et al.*, 2002); here the crystal structure of 6-(3-iodopropyl)benzo[*f*][1,7]naphthyridin-6-ium iodide, (I), is reported.



(I)

Similar to the case of other quaternary azaaromatic salts with two unprotonated, mono- or diprotonated aza-aromatic N atoms, *e.g.* $C_{12}H_9N_2^+\cdot Cl^-$ (Hensen *et al.*, 2000),

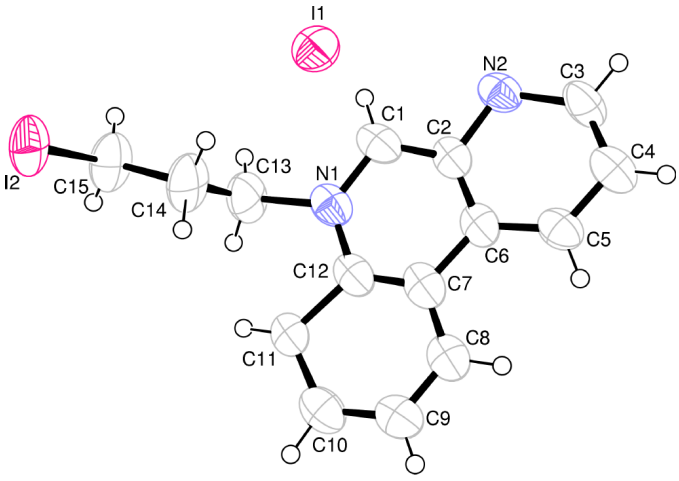


Figure 1
The constituent ions of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

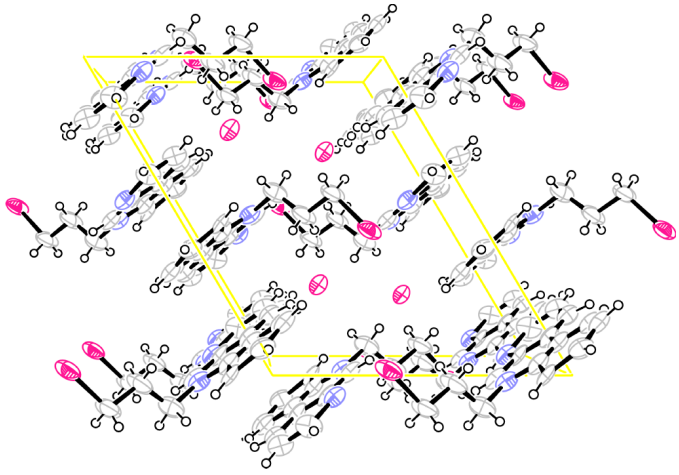


Figure 2
The unit-cell contents, viewed along *b*.

$3C_{12}H_9N_2^+\cdot 2Cl^-\cdot HCl\cdot Cl^-\cdot CHCl_3$ (Hensen *et al.*, 2000), $2C_{12}H_9N_2^+\cdot I_2Cl^-\cdot Cl_2I^-$ (Wang *et al.*, 1999*a*), $2C_{12}H_{10}N_2^+\cdot ClICl^-\cdot Cl^-$ (Wang *et al.*, 1999*b*), $C_{12}H_9N_2^+\cdot Br^-$ (Marciniak *et al.*, 2002*a*), $C_{14}H_{13}N_2O^+\cdot Br^-$ (Marciniak *et al.*, 2002*b*) and $C_{14}H_{13}N_2^+\cdot I^-$ (Marciniak *et al.*, 2002), the crystal packing of the title compound is stabilized by several short I···H—C contacts.

Experimental

The title compound was synthesized by treatment of a solution of benzo[*f*]-1,7-naphthyridine (0.9 g, 5 mmol) in 2-propanol (12 ml) with 1,3-diiodopropane (19.2 g, 75 mmol). After refluxing for 72 h, the reaction mixture was cooled and the resulting two layers were separated. The upper layer was evaporated to give the crude product, which was thoroughly washed with hot *n*-heptane followed by hot ethanol. The melting point of the final product, measured by means of an electrothermal IA 910 apparatus, was 446–447 K. Tablet-like optically clear pale-yellow crystals of the title compound were grown from solution by slow evaporation of the dimethylformamide–tetrahydrofuran mixture used as a solvent at a constant temperature of 293 K.

Crystal data

$C_{15}H_{14}IN_2^+\cdot I^-$
M_r = 475.8
Monoclinic, $P2_1/c$
a = 10.896 (1) Å
b = 12.547 (2) Å
c = 13.454 (2) Å
β = 120.71 (2)°
V = 1581.4 (5) Å^3
Z = 4
D_x = 2.000 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 27 reflections
θ = 3–22°
μ = 3.97 mm^{-1}
T = 293 (2) K
Tablet, clear pale yellow
0.29 × 0.15 × 0.09 mm

Data collection

DARCH-1 diffractometer
ω–2θ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
T_{min} = 0.491, T_{max} = 0.702
3784 measured reflections
3622 independent reflections
3075 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.5°
$h = -14 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = 0 \rightarrow 17$
3 standard reflections every 100 reflections
intensity decay: negligible

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.095
S = 1.19
3622 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 1.109P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.012
$\Delta\rho_{max}$ = 1.36 e Å^{-3}
$\Delta\rho_{min}$ = −1.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···I1^{i}	0.93	3.02	3.919 (7)	164
C11—H11···I1^{ii}	0.93	3.09	3.882 (4)	144
C13—H13*B*···I1^{ii}	0.97	3.19	4.147 (5)	167
C14—H14*B*···I1	0.97	3.01	3.920 (7)	157

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

The positions of the H atoms were calculated and refined using SHELXL97 (Sheldrick, 1997) constraints. The maximum and minimum electron-density peaks were located 0.44 and 0.41 Å from atom C13, respectively.

Data collection: *DARCH Package* (Burevestnik, 1991); cell refinement: *DARCH Package*; data reduction: *DARCH package*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *PLATON* (Spek, 2000); software used to prepare material for publication: *SHELXL*97.

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