

## 1-Allyl-4-aminopyridinium bromide

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## Key indicators

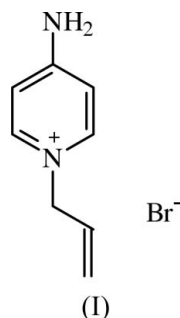
Single-crystal X-ray study  
 $T = 293$  K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å  
 $R$  factor = 0.064  
 $wR$  factor = 0.164  
 Data-to-parameter ratio = 23.0

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

The asymmetric unit of the title structure,  $\text{C}_8\text{H}_{11}\text{N}_2^+\cdot\text{Br}^-$ , contains two independent cations and two anions. In one cation, the dihedral angle between the mean planes of the pyridinium ring and the allyl group is  $86.43(6)^\circ$ , while in the other cation this dihedral angle is  $72.93(7)^\circ$ . In the crystal structure, anions and cations are linked *via* intermolecular  $\text{N}-\text{H}\cdots\text{Br}$  hydrogen bonds, forming one-dimensional chains along [010].

## Comment

In human peripheral mononuclear cells isolated from healthy volunteers, derivatives of pyridinium compounds have been identified. 4-Aminopyridine (4AP) has been found to be an efficient drug, affecting potassium permeability and capable of provoking membrane depolarization (Grissmer *et al.*, 1992) and is also able to induce an increase in intracellular calcium influx through modulation of the activity of purinergic cationic channels (Lajdova *et al.*, 2004). We report here the crystal structure of the title pyridinium derivative, (I).



The asymmetric unit of (I) consists of two independent pyridinium cations (labelled *A* and *B*) and two bromide anions (Fig. 1). The bond lengths and angles within the pyridinium ring are comparable with those in reported structures (Seethalakshmi, Kaliannan *et al.*, 2006; Seethalakshmi *et al.*, 2006*a,b,c*). The dihedral angle between the mean planes of the pyridinium ring and allyl group is  $86.4(6)^\circ$  for cation *A* and  $72.93(7)^\circ$  for cation *B*.

In the crystal structure, atom N2 of each cation acts as a donor for an intermolecular  $\text{N}-\text{H}\cdots\text{Br}$  hydrogen bond with two different symmetry-related bromide anions (Table 1 and Fig. 2). These hydrogen bonds link cations *A* and *B* into a one-dimensional chain parallel to the *b* axis, which can be described by graph-set motif *C*(5).

## Experimental

A solution of 4-aminopyridine (1.175 g, 25 ml) and allyl bromide (1.51 g, 25 ml) in dry acetone (20 ml) was stirred for 44 h at room

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temperature (303 K). The solid that separated was filtered, washed with dry acetone and dried in a vacuum to give the stable salt, (I), which was recrystallized from an aqueous ethanol (80% v/v) solution (yield 74%).

#### Crystal data

$C_8H_{11}N_2^+ \cdot Br^-$	$V = 889.6 (5) \text{ \AA}^3$
$M_r = 215.10$	$Z = 4$
Triclinic, $P\bar{1}$	$D_x = 1.606 \text{ Mg m}^{-3}$
$a = 6.9085 (19) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.179 (3) \text{ \AA}$	$\mu = 4.56 \text{ mm}^{-1}$
$c = 14.186 (4) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 90.096 (4)^\circ$	Block, colourless
$\beta = 97.446 (4)^\circ$	$0.49 \times 0.32 \times 0.26 \text{ mm}$
$\gamma = 94.164 (4)^\circ$	

#### Data collection

Bruker APEX-2 CCD area-detector diffractometer	9293 measured reflections
$\varphi$ and $\omega$ scans	4585 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3443 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.171$ , $T_{\max} = 0.307$	$R_{\text{int}} = 0.035$
	$\sigma_{\text{max}} = 28.9^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 8.4291P]$
$R[F^2 > 2\sigma(F^2)] = 0.064$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.164$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 1.98 \text{ e \AA}^{-3}$
4585 reflections	$\Delta\rho_{\text{min}} = -1.25 \text{ e \AA}^{-3}$
199 parameters	
H-atom parameters constrained	

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2A-H2A1 \cdots Br1^i$	0.86	2.57	3.411 (6)	165
$N2A-H2A2 \cdots Br2^{ii}$	0.86	2.58	3.399 (6)	159
$N2B-H2B1 \cdots Br2^{iii}$	0.86	2.54	3.386 (5)	167
$N2B-H2B2 \cdots Br1^{iii}$	0.86	2.51	3.354 (6)	169

Symmetry codes: (i)  $-x+1, -y+2, -z$ ; (ii)  $-x+1, -y+1, -z$ ; (iii)  $-x+1, -y+1, -z+1$ .

H atoms were positioned geometrically ( $C-H = 0.93-0.99 \text{ \AA}$  and  $N-H = 0.86 \text{ \AA}$ ) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ . The largest peak in the final difference Fourier is  $0.92 \text{ \AA}$  from atom Br1 and the deepest hole is  $0.79 \text{ \AA}$  from atom H4A.

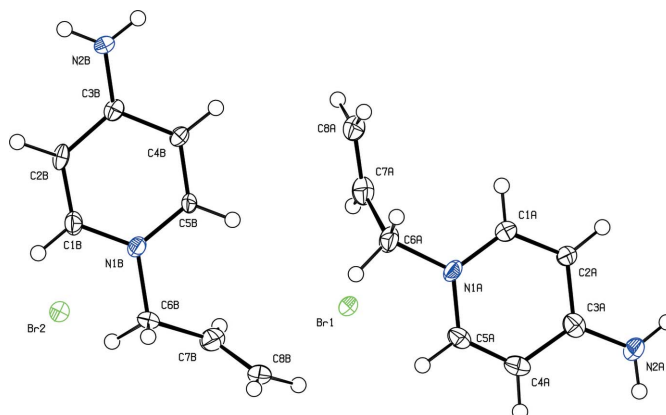
Data collection: APEX2 (Bruker, 2006); cell refinement: APEX2; data reduction: APEX2; program(s) used to solve structure: SHELXL97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PARST (Nardelli, 1995).

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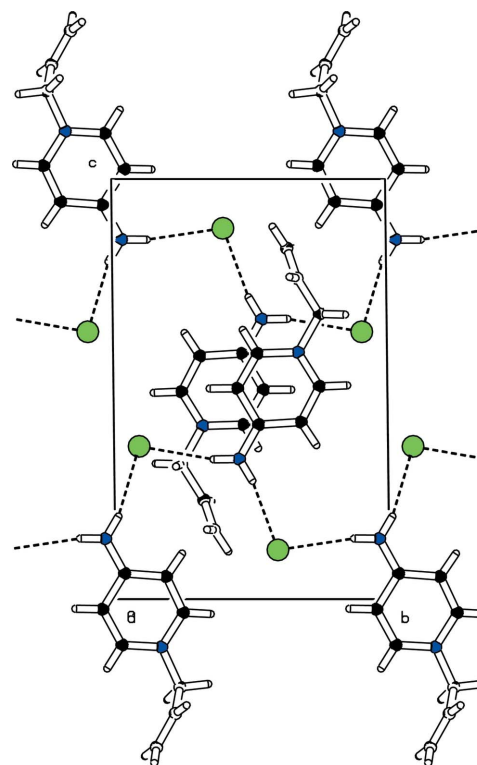
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**Figure 1**

View of the asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.



**Figure 2**

The crystal structure of (I), viewed along the  $a$  axis. Intermolecular  $N-H \cdots Br$  hydrogen bonds are indicated by dashed lines.

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