

2-Amino-(1-methylphenyl)pyridinium bromide

T. Seethalakshmi,^a
 P. Venkatesan,^b Ray J. Butcher,^c
 M. Nallu^d and P. Kaliannan^{a*}

^aSchool of Physics, Bharathidasan University, Tiruchirappalli 620 024, India, ^bSchool of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, India, ^cDepartment of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, and ^dDepartment of Chemistry, Bharathidasan Institute of Technology, Tiruchirappalli 620 024, India

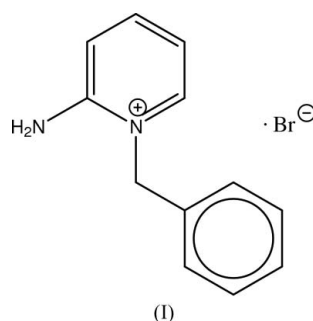
Correspondence e-mail: kal_44in@yahoo.co.in

In the cation of the title compound, $C_{12}H_{13}N_2^+ \cdot Br^-$, the dihedral angle between the pyridine and benzene rings is $89.2(1)^\circ$. In the crystal structure, anions and cations are interconnected by $N-H \cdots Br$ hydrogen bonds, forming clusters about crystallographic twofold rotation axes.

Received 4 August 2006
 Accepted 16 August 2006

Comment

2-Aminopyridine is a commonly used drug for the treatment of neurological ailments such as multiple sclerosis, with tests showing that 2-aminopyridine improves motor functions in multiple sclerosis patients (Schwid *et al.*, 1997).



Key indicators

Single-crystal X-ray study
 $T = 103$ K
 Mean $\sigma(C-C) = 0.002$ Å
 R factor = 0.021
 wR factor = 0.053
 Data-to-parameter ratio = 23.9

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

As an extension of our study of hydrogen-bonding patterns of pyridinium derivatives (Seethalakshmi *et al.*, 2006,

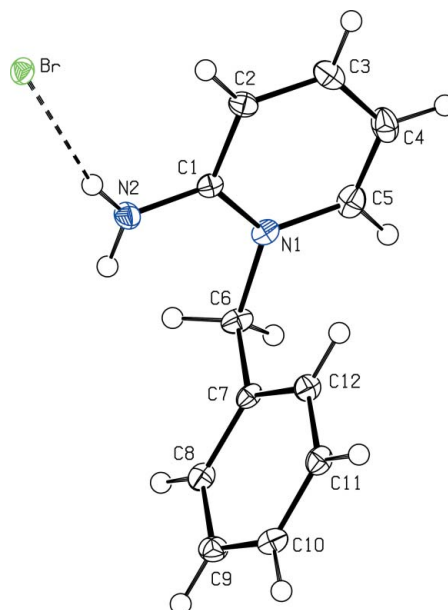


Figure 1
 View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

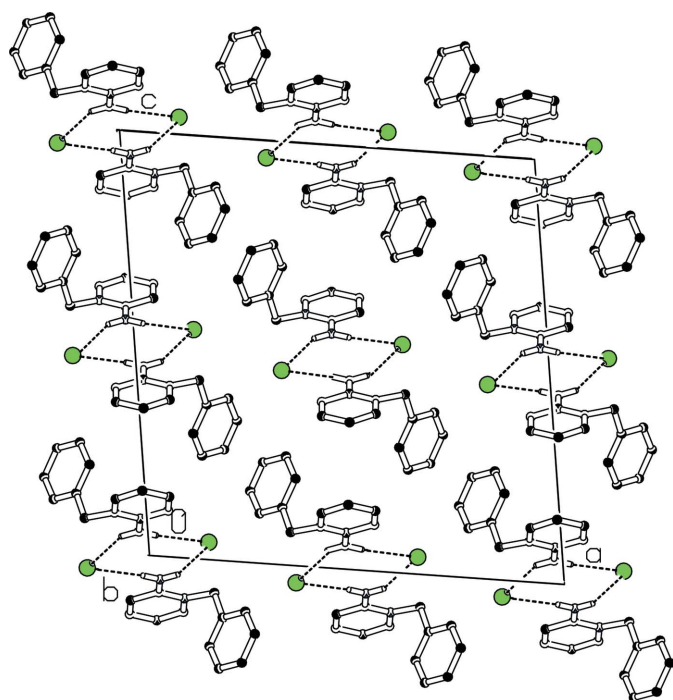


Figure 2
Part of the crystal structure of (I), viewed along the *b* axis. Intermolecular N—H...Br hydrogen bonds are indicated by dashed lines. Only H atoms involved in the hydrogen bonding have been included.

Seethalakshmi *et al.*, 2006*a,b*), the X-ray crystal structure determination of (I), has been undertaken. A view of the cation and anion of (I), with the atomic numbering scheme is shown in Fig. 1. The bond lengths and angles within the pyridinium ring are comparable with those reported for related structures (Seethalakshmi *et al.*, 2006, 2006*a,b*). In (I), the dihedral angle between the planes of the pyridine and benzene rings is 89.2 (1)°.

In the crystal structure, adjacent pyridinium cations are interconnected by bromide anions through intermolecular N—H...Br hydrogen bonds, resulting in the formation of clusters about twofold rotation axes (Table 1 and Fig. 2)

Experimental

A solution of 2-aminopyridine (1.175 g, 25 ml), benzyl bromide (2.13 g, 25 ml) in dry acetone was stirred for 44 h at room temperature (303 K). The solid that separated was filtered, washed with dry acetone and dried in vacuum to give the stable salt, (I), which was recrystallized from an aqueous ethanol (80% *v/v*) solution.

Crystal data

$C_{12}H_{13}N_2^+ \cdot Br^-$
 $M_r = 265.15$
Monoclinic, $C2/c$
 $a = 18.4425$ (10) Å
 $b = 6.5063$ (4) Å
 $c = 18.8979$ (11) Å
 $\beta = 98.0230$ (10)°
 $V = 2245.4$ (2) Å³

$Z = 8$
 $D_x = 1.569$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 3.63$ mm⁻¹
 $T = 103$ (2) K
Block, colourless
 $0.56 \times 0.50 \times 0.50$ mm

Data collection

Bruker SMART CCD
diffractometer
 φ and ω scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $T_{\min} = 0.138$, $T_{\max} = 0.163$

12321 measured reflections
3270 independent reflections
3025 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.016$
 $\theta_{\text{max}} = 30.8^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.021$
 $wR(F^2) = 0.053$
 $S = 1.07$
3270 reflections
137 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 2.2052P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.81$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³
Extinction correction: SHELXL97
Extinction coefficient: 0.0006 (2)

Table 1

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
N2—H2B...Br ⁱ	0.88	2.59	3.3962 (11)	153
N2—H2C...Br	0.88	2.48	3.3466 (11)	167

Symmetry code: (i) $-x, -y + 1, -z + 1$.

All the H atoms were positioned geometrically (C—H = 0.95–0.99 Å and N—H = 0.88 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL (Bruker, 1999).

TS thanks Professor V. Parthasarathi, School of Physics, Bharathidasan University, Tiruchirappalli, and Dr S. Thamocharan, Molecular Biophysics Unit, Indian Institute of Science, Bangalore, for their generous help.

References

- Bruker (1998). SMART. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). SAINT-Plus and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
Schwid, S. R., Petrie, M. D., Mc Dermott, M. P., Tierney, D. S., Mason, D. H. & Goddman, A. D. (1997). *Neurology*, **48**, 817–821.
Seethalakshmi, T., Kaliannan, P., Venkatesan, P., Fronczek, F. R. & Thamocharan, S. (2006). *Acta Cryst.* **E62**, o2353–o2355.
Seethalakshmi, T., Venkatesan, P., Fronczek, F. R., Kaliannan, P. & Thamocharan, S. (2006*a*). *Acta Cryst.* **E62**, o2560–o2562.
Seethalakshmi, T., Venkatesan, P., Fronczek, F. R., Kaliannan, P. & Thamocharan, S. (2006*b*). *Acta Cryst.* **E62**, o3389–o3390.
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
Sheldrick, G. M. (1997). SHELXL97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.