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4-Amino-(1-methylphenyl)pyridinium bromide

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Key indicators

Single-crystal X-ray study
T = 115 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.050
Data-to-parameter ratio = 26.0

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

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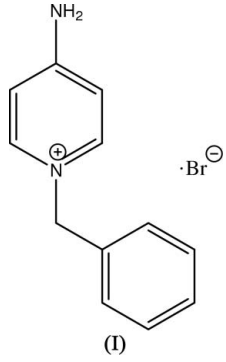
In the cation of the title compound, $C_{12}H_{13}N_2^+\cdot Br^-$, the dihedral angle between the pyridine and benzene rings is 80.0 (1)°. The anions and cations are connected by intermolecular N—H···Br hydrogen bonds, forming one-dimensional chains along [100].

Comment

It is well known that pyridinium derivatives often exhibit antibacterial and antifungal activities (Akkurt *et al.*, 2005). In a continuation of our work on the study of pyridinium derivatives, the structure determination of the title compound, (I), has been undertaken.



(I)

A perspective view of the molecular structure of (I) is shown in Fig. 1. The bond lengths and angles within the pyridinium ring are normal and comparable with those reported for related structures (Sundar *et al.*, 2004*a*,*b*, 2005, 2006, 2006*a*,*b*). In (I), the dihedral angle between the planes of the pyridine and benzene rings is 80.0 (1)°. In related structures, this angle is 85.0 (1)° for 2-amino-1-(4-nitrobenzyl)pyridinium bromide (Sundar *et al.*, 2006*a*), 88.7 (1)° for 3-amino-1-(4-nitrobenzyl)pyridinium bromide (Sundar *et al.*, 2006*b*) and 89.2 (1)° for 4-amino-1-(4-nitrobenzyl)pyridinium bromide (Sundar, Parthasarathi, Ravikumar *et al.*, 2006).

In the crystal structure, intermolecular N—H···Br hydrogen bonds, connect the cations and anions (Fig. 2 and Table 1). The pyridinium cations are stacked along the shortest cell axis. In addition to these interactions, a weak intermolecular C—H···Br interaction also is observed involving the H atom bonded to C2 and Br1 [C2···Br1 = 3.705 (2) Å and C2—H2···Br1 = 142°].

Experimental

A solution of 4-aminopyridine (2.35 g, 25 ml) and benzyl bromide (4.28 g, 25 ml) in acetone was stirred at room temperature (303 K) for

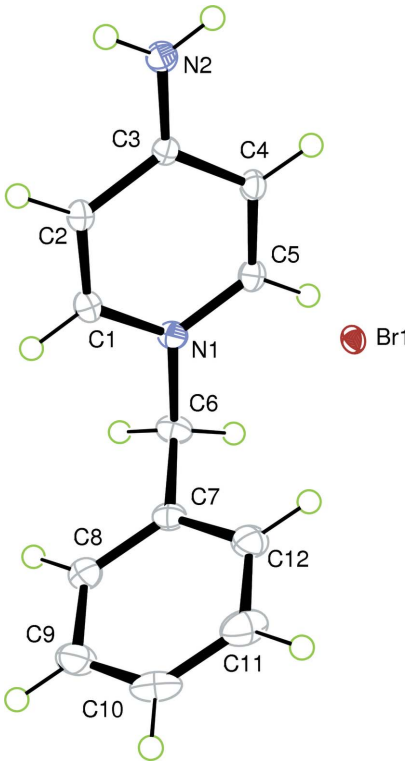


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

1–2 h. 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 (m.p. 458–460 K).

Crystal data

$C_{12}H_{13}N_2^+\cdot Br^-$
M_r = 265.15
Orthorhombic, $P2_12_12_1$
a = 6.4916 (5) Å
b = 7.4037 (5) Å
c = 23.818 (2) Å
V = 1144.74 (15) Å^3
Z = 4
D_x = 1.539 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.56 mm^{-1}
T = 115 (2) K
Fragment, colourless
0.30 × 0.22 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer with an Oxford Cryostream cooler
ω scans with κ offsets
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.382, T_{max} = 0.493
24420 measured reflections
3742 independent reflections
3593 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 31.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.050
S = 1.07
3742 reflections
144 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0176P)^2 + 0.8443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), 1543 Friedel pairs
Flack parameter: 0.025 (8)

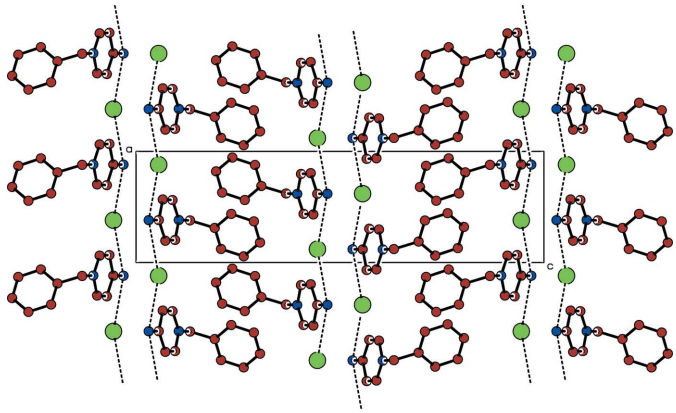


Figure 2
The crystal structure of (I), viewed along the *b* axis. The dashed lines indicate the N—H···Br hydrogen bonds. H atoms have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···Br1^{i}	0.82 (3)	2.78 (3)	3.5116 (18)	150 (2)
N2—H22···Br1^{ii}	0.87 (3)	2.72 (3)	3.5201 (18)	154 (2)

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

All H atoms, except amino H atoms, were placed in geometrically idealized positions (C—H = 0.95–0.99 Å) and were constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). The positions of amino H atoms were obtained from a difference map and refined freely along with their isotropic displacement parameters.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Version 1.07; Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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References

Akkurt, M., Karaca, S., Jarrahpour, A. A., Zarei, M. & Büyükgüngör, O. (2005). *Acta Cryst.* E**61**, o776–o778.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*, University of Göttingen, Germany.
Sundar, T. V., Parthasarathi, V., Ravikumar, K., Venkatesan, P. & Nallu, M. (2006). *Acta Cryst.* E**62**, o1118–o1120.
Sundar, T. V., Parthasarathi, V., Sarkunam, K., Nallu, M., Walfort, B. & Lang, H. (2004*a*). *Acta Cryst.* C**60**, o464–o466.

Sundar, T. V., Parthasarathi, V., Sarkunam, K., Nallu, M., Walfort, B. & Lang, H. (2004*b*). *Acta Cryst.* E**60**, o2345–o2346.
Sundar, T. V., Parthasarathi, V., Sarkunam, K., Nallu, M., Walfort, B. & Lang, H. (2005). *Acta Cryst.* E**61**, o889–o891.
Sundar, T. V., Parthasarathi, V., Sridhar, B., Venkatesan, P. & Nallu, M. (2006*a*). *Acta Cryst.* E**62**, o74–o76.
Sundar, T. V., Parthasarathi, V., Sridhar, B., Venkatesan, P. & Nallu, M. (2006*b*). *Acta Cryst.* E**62**, o482–o484.