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Key indicators

Single-crystal X-ray study
 $T = 294\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$
 R factor = 0.056
 wR factor = 0.157
Data-to-parameter ratio = 14.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

1,1'-Ethylenebis(4-aminopyridinium) dibromide

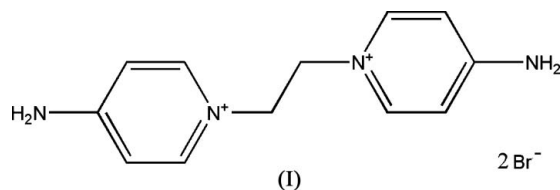
In the title compound, $\text{C}_{12}\text{H}_{16}\text{N}_4^{2+} \cdot 2\text{Br}^-$, the molecule has a centre of symmetry at the mid-point of the central C—C bond and a mirror plane passes through the amino N atom, the attached C atom, the ring N atom, and the linking chain C atom; the Br anion lies on a position of site symmetry m . The two pyridyl rings are parallel to each other.

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Comment

N-(2-Bromoethyl)pyridinium cations and 1,1'-ethylenebispyridinium dications are potential sources of *N*-vinylpyridinium cations *via* base-catalysed elimination reactions (Katritzky & Rubio, 1983). Bunting *et al.*, (1992) have conducted research on the elimination reaction of 1,1'-ethylenebis(4-aminopyridinium) dibromide, (I), in an aqueous base medium. Here we report the crystal structure of (I).



The molecular structure of (I) is shown in Fig. 1. The molecule has a centre of symmetry at the mid-point of the C6—C6(1 - x , - y , 1 - z) bond and a mirror plane passes through atoms C1, N2 and C6. Atom Br1 lies on a position of site symmetry m . The two pyridyl rings are parallel to each other. The bond N1—C1 is short enough [1.325 (12) Å] to indicate significant double-bond character. The planar geometry around the amino N atom suggests strong conjugation with the π -system of the pyridyl ring. The $\text{N}^+ \cdots \text{N}^+$ distance in (I) is 3.740 (1) Å, similar to the value previously reported (*ca* 3.75 Å) in the 1,2-bis(pyridinium)ethane dication (Loeb & Wisner, 1998). The bond lengths and angles are unexceptional. The molecular structure is stabilized by an intermolecular N—H \cdots Br hydrogen bond (Table 1).

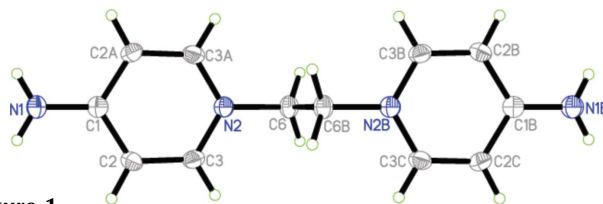


Figure 1
View of the structure of the cation of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The bromide ions have been omitted for clarity. [Symmetry codes: (A) $x, -y, z$; (B) $1 - x, -y, 1 - z$; (C) $1 - x, y, 1 - z$.]

Experimental

1,1'-Ethylenebis(4-aminopyridinium) dibromide was prepared according to the method of Bunting (1992). Single crystals suitable for analysis were grown by evaporation of an ethanol solution.

Crystal data

$C_{12}H_{16}N_4^{2+} \cdot 2Br^-$	$D_x = 1.799 \text{ Mg m}^{-3}$
$M_r = 376.11$	Mo $K\alpha$ radiation
Monoclinic, $C2/m$	Cell parameters from 1061 reflections
$a = 13.121 (4) \text{ \AA}$	$\theta = 3.2\text{--}26.2^\circ$
$b = 6.4876 (19) \text{ \AA}$	$\mu = 5.83 \text{ mm}^{-1}$
$c = 8.406 (2) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\beta = 104.023 (5)^\circ$	Block, colorless
$V = 694.2 (4) \text{ \AA}^3$	$0.32 \times 0.22 \times 0.18 \text{ mm}$
$Z = 2$	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	758 independent reflections
φ and ω scans	638 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.033$
$T_{\text{min}} = 0.214$, $T_{\text{max}} = 0.350$	$\theta_{\text{max}} = 26.2^\circ$
1850 measured reflections	$h = -16 \rightarrow 14$
	$k = -8 \rightarrow 7$
	$l = -10 \rightarrow 7$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0778P)^2 + 6.17P]$
$R[F^2 > 2\sigma(F^2)] = 0.056$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.157$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.11$	$\Delta\rho_{\text{max}} = 1.52 \text{ e \AA}^{-3}$
758 reflections	$\Delta\rho_{\text{min}} = -0.93 \text{ e \AA}^{-3}$
52 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1A \cdots Br1^i$	0.83 (8)	2.70 (8)	3.516 (3)	166 (7)

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

Atom H1A was located in a difference Fourier map and refined freely; the final $N1-H1A$ bond length is $0.83 (8) \text{ \AA}$; the $U_{\text{iso}}(\text{H})$ value was set equal to $1.5U_{\text{eq}}(\text{N})$. Other H atoms were positioned geometrically and constrained to ride on their parent atoms [$C-H = 0.93 \text{ \AA}$ for aromatic and 0.97 \AA for CH_2 groups, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. The maximum residual electron-density peak is located 0.87 \AA from atom Br1.

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

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