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Hexane-1,6-diyldipyridinium dibromide

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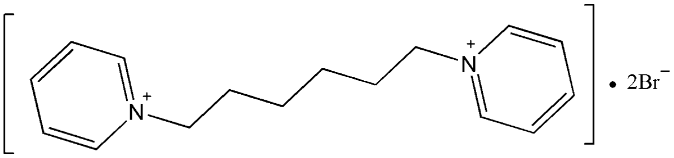
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.035; wR factor = 0.082; data-to-parameter ratio = 18.0.

The cation of the title compound, $C_{16}H_{22}N_2^{+}\cdot 2Br^-$, has a crystallographic inversion centre.

Related literature

For general background, see: Cong *et al.* (2007); Allen *et al.* (1987). For related literature, see: Ji *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{22}N_2^{2+}\cdot 2Br^-$
M_r = 402.16
Triclinic, $P\bar{1}$
a = 7.4750 (15) Å
b = 7.9320 (16) Å
c = 8.3450 (17) Å
α = 94.12 (3)°
β = 115.64 (3)°
γ = 105.91 (3)°
V = 418.5 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 4.84 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.326, T_{max} = 0.617
1774 measured reflections
1639 independent reflections
1155 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.082
S = 1.04
1639 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2253).

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supplementary materials

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Hexane-1,6-diyldipyridinium dibromide

R.-J. Ni, Y. Huang and **C. Yao**

Comment

The title compound, (I), with cucurbit[6,7,8]urils, can be utilized to form host–guest complexes (Cong *et al.*, 2007), which are of wide current interest for application in molecular identification and molecular self-assembly. A relative crystal structure has already been reported (Ji *et al.*, 2006). We report herein the crystal structure of the title compound, (I).

The asymmetric unit of the title compound, (I), contains one half molecule (Fig. 1), in which the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

Experimental

For the preparation of the title compound, (I), 1,6-dibromohexane (12.2 g, 50 mmol) was added to 2-propanol solution (50 ml) of pyridine (9.5 g, 120 mmol) at 353 K. After stirring for 12 h, two layers were formed. The top layer containing the unreacted starting materials was decanted. The bottom layer, a white solid phase, was recrystallized by the addition of ethanol. Then, the crystals of (I) were obtained by evaporating the solvent slowly at room temperature for about 7 d.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$.

Figures

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code (A): 2 − *x*, −*y*, −*z*].

Hexane-1,6-diyldipyridinium dibromide

Crystal data

$C_{16}H_{22}N_2^{2+}\cdot 2Br^-$

$M_r = 402.16$

Triclinic, $P\overline{1}$

Hall symbol: -P 1

$a = 7.4750$ (15) Å

$b = 7.9320$ (16) Å

$c = 8.3450$ (17) Å

$Z = 1$

$F_{000} = 202$

$D_x = 1.596$ Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 25 reflections

θ = 10–13°

μ = 4.84 mm^{-1}

α = 94.12 (3)°
β = 115.64 (3)°
γ = 105.91 (3)°
V = 418.5 (2) Å^3

T = 298 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 298(2) K
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.326, T_{max} = 0.617
1774 measured reflections
1639 independent reflections
1155 reflections with $I > 2\sigma(I)$

R_{int} = 0.054
θ_{max} = 26.0°
θ_{min} = 2.7°
$h = -9 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = 0 \rightarrow 10$
3 standard reflections
every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.082
S = 1.04
1639 reflections
91 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.3P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\text{max}}$ = 0.001
$\Delta\rho_{\text{max}}$ = 0.65 e Å^{-3}
$\Delta\rho_{\text{min}}$ = −0.43 e Å^{-3}
Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Br	0.04735 (6)	0.78621 (5)	0.21069 (5)	0.04621 (16)
N	0.8561 (4)	1.2391 (4)	0.2347 (4)	0.0336 (6)
C1	0.5568 (6)	1.0791 (5)	0.2592 (5)	0.0491 (10)
H1A	0.4965	1.0004	0.3138	0.059*
C2	0.4352 (6)	1.1500 (5)	0.1262 (6)	0.0477 (10)
H2A	0.2912	1.1182	0.0875	0.057*
C3	0.5292 (6)	1.2688 (5)	0.0511 (6)	0.0506 (10)
H3A	0.4494	1.3204	−0.0374	0.061*
C4	0.7412 (6)	1.3119 (5)	0.1062 (5)	0.0427 (9)
H4A	0.8045	1.3915	0.0542	0.051*
C5	0.7674 (6)	1.1244 (5)	0.3114 (5)	0.0423 (9)
H5A	0.8498	1.0752	0.4009	0.051*
C6	1.0866 (5)	1.2841 (5)	0.2952 (5)	0.0400 (8)
H6A	1.1207	1.3419	0.2086	0.048*
H6B	1.1203	1.1743	0.2976	0.048*
C7	1.2187 (5)	1.4073 (5)	0.4823 (5)	0.0395 (8)
H7A	1.1776	1.3533	0.5673	0.047*
H7B	1.1927	1.5206	0.4779	0.047*
C8	1.4535 (5)	1.4423 (5)	0.5498 (5)	0.0383 (8)
H8A	1.5296	1.5000	0.6782	0.046*
H8B	1.4750	1.3278	0.5382	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0391 (2)	0.0478 (2)	0.0494 (2)	0.00794 (16)	0.02235 (17)	0.01417 (17)
N	0.0231 (14)	0.0321 (15)	0.0387 (16)	0.0015 (11)	0.0143 (12)	0.0007 (12)
C1	0.036 (2)	0.053 (2)	0.054 (2)	−0.0008 (18)	0.0275 (19)	0.006 (2)
C2	0.0256 (18)	0.049 (2)	0.059 (2)	0.0040 (17)	0.0202 (18)	−0.0100 (19)
C3	0.038 (2)	0.048 (2)	0.055 (2)	0.0176 (18)	0.0123 (18)	0.0030 (19)
C4	0.041 (2)	0.0343 (19)	0.050 (2)	0.0070 (16)	0.0219 (18)	0.0098 (17)
C5	0.0335 (19)	0.046 (2)	0.042 (2)	0.0064 (16)	0.0184 (16)	0.0095 (17)
C6	0.0251 (17)	0.043 (2)	0.048 (2)	0.0026 (15)	0.0204 (15)	−0.0018 (17)
C7	0.0226 (16)	0.042 (2)	0.048 (2)	0.0016 (15)	0.0189 (15)	0.0013 (17)
C8	0.0271 (17)	0.041 (2)	0.044 (2)	0.0064 (15)	0.0175 (15)	0.0052 (16)

Geometric parameters (Å, °)

N—C4	1.335 (5)	C5—H5A	0.9300
N—C5	1.341 (4)	C6—C7	1.512 (5)
N—C6	1.495 (4)	C6—H6A	0.9700
C1—C2	1.368 (6)	C6—H6B	0.9700
C1—C5	1.368 (5)	C7—C8	1.526 (4)
C1—H1A	0.9300	C7—H7A	0.9700
C2—C3	1.370 (6)	C7—H7B	0.9700

C2—H2A	0.9300	C8—C8^{i}	1.507 (7)
C3—C4	1.375 (5)	C8—H8A	0.9700
C3—H3A	0.9300	C8—H8B	0.9700
C4—H4A	0.9300		

C4—N—C5	120.8 (3)	N—C6—C7	111.4 (3)
C4—N—C6	120.4 (3)	N—C6—H6A	109.3
C5—N—C6	118.8 (3)	C7—C6—H6A	109.3
C2—C1—C5	119.7 (4)	N—C6—H6B	109.3
C2—C1—H1A	120.1	C7—C6—H6B	109.3
C5—C1—H1A	120.1	H6A—C6—H6B	108.0
C1—C2—C3	118.8 (3)	C6—C7—C8	111.4 (3)
C1—C2—H2A	120.6	C6—C7—H7A	109.4
C3—C2—H2A	120.6	C8—C7—H7A	109.4
C2—C3—C4	120.2 (4)	C6—C7—H7B	109.4
C2—C3—H3A	119.9	C8—C7—H7B	109.4
C4—C3—H3A	119.9	H7A—C7—H7B	108.0
N—C4—C3	119.8 (4)	C8^{i}—C8—C7	114.5 (4)
N—C4—H4A	120.1	C8^{i}—C8—H8A	108.6
C3—C4—H4A	120.1	C7—C8—H8A	108.6
N—C5—C1	120.6 (4)	C8^{i}—C8—H8B	108.6
N—C5—H5A	119.7	C7—C8—H8B	108.6
C1—C5—H5A	119.7	H8A—C8—H8B	107.6

C5—C1—C2—C3	−1.5 (6)	C6—N—C5—C1	−179.7 (3)
C1—C2—C3—C4	1.5 (6)	C2—C1—C5—N	0.7 (6)
C5—N—C4—C3	−0.2 (5)	C4—N—C6—C7	106.6 (4)
C6—N—C4—C3	179.7 (3)	C5—N—C6—C7	−73.6 (4)
C2—C3—C4—N	−0.7 (6)	N—C6—C7—C8	175.9 (3)
C4—N—C5—C1	0.2 (5)	C6—C7—C8—C8^{i}	70.2 (5)

Symmetry codes: (i) $-x+3, -y+3, -z+1$.

Fig. 1