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1-(4-Cyanobenzyl)-4-methylpyridinium bromide

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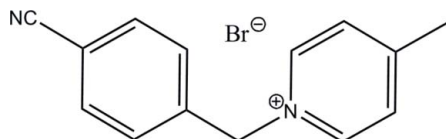
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.066; wR factor = 0.204; data-to-parameter ratio = 14.8.

In the title compound, $\text{C}_{14}\text{H}_{13}\text{N}_2^+\cdot\text{Br}^-$, the 1-(4-cyanobenzyl)-4-methylpyridinium cation has a Δ -shaped conformation, and the dihedral angle between the benzene and pyridinium rings is 75.8 (2)°. In the crystal, two cations form a dimer through π - π interactions between pyridine rings [the centroid-centroid distance is 3.685 (1) Å].

Related literature

For cations with similar geometry, see: Liu *et al.* (2007, 2008).

Experimental

Crystal data

 $\text{C}_{14}\text{H}_{13}\text{N}_2^+\cdot\text{Br}^-$ $M_r = 289.17$

Monoclinic, $P2_1/c$
 $a = 12.967$ (5) Å
 $b = 8.217$ (4) Å
 $c = 12.260$ (5) Å
 $\beta = 96.900$ (5)°
 $V = 1296.8$ (10) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 3.15$ mm⁻¹
 $T = 296$ K
 $0.24 \times 0.20 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.493$, $T_{\max} = 0.601$

6270 measured reflections
 2298 independent reflections
 1945 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.106$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.066$
 $wR(F^2) = 0.204$
 $S = 1.04$
 2298 reflections

155 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.84$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.82$ e Å⁻³

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); 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: BQ2140).

References

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 Liu, G.-X. (2007). *Acta Cryst.* E63, o704–o706.
 Liu, G.-X., Xu, H., Ren, X.-M. & Sun, W.-Y. (2008). *CrystEngComm*, 10, 1574–1582.
 Sheldrick, G. M. (2008). *Acta Cryst.* A64, 112–122.

supplementary materials

Acta Cryst. (2009). E65, o1453 [doi:10.1107/S1600536809020054]

1-(4-Cyanobenzyl)-4-methylpyridinium bromide

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Comment

The asymmetric unit of (I) contains one cation and one Br anion (Fig. 1). The cation has a Λ -shaped conformation, and the dihedral angles formed by the C5/C8/N2 plane with the benzene and pyridinium rings are $61.19(2)^\circ$ and $72.88(2)^\circ$, respectively ($75.8(2)^\circ$ between the benzene and pyridinium rings). The geometry of the cation is similar to the one observed in Liu *et al.* (2008) and Liu *et al.* (2007). Two cations form a dimer through π - π interaction between pyridine rings, the distance of centroid-to-centroid is 3.685\AA , which further are linked into one dimensional chain by the π - π interaction between benzene ring, the distance of centroid-to-centroid is 4.242\AA . A three-dimensional supramolecular structure was packed via Van der Waals forces (Fig. 2).

Experimental

4-cyanobenzyl bromide (10 mmol, 1.96 g) and 4-methylpyridine (20 mmol, 1.88 g) were added to 40 ml of acetone. After stirring and refluxing for 12 h, the mixture was filtered, and the clear solution was allowed to evaporate slowly under inert atmosphere. Block crystals of the title compound were obtained after 3 days. The crystals were filtered, washed by acetone and dried in air.

Refinement

H atoms were positioned geometrically, with C—H = 0.93\AA , 0.96\AA and 0.97\AA for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl H and $x = 1.2$ for other H atoms. The deepest hole is located 1.12\AA from atom C16.

Figures

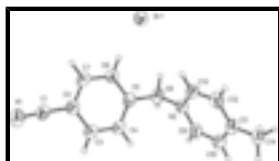


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

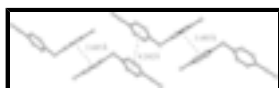


Fig. 2. One dimensional chain is formed by π - π interaction along the a -axis.

1-(4-Cyanobenzyl)-4-methylpyridinium bromide

Crystal data

$\text{C}_{14}\text{H}_{13}\text{N}_2^+\cdot\text{Br}^-$

$F_{000} = 584$

supplementary materials

$M_r = 289.17$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.967 (5) \text{ \AA}$

$b = 8.217 (4) \text{ \AA}$

$c = 12.260 (5) \text{ \AA}$

$\beta = 96.900 (5)^\circ$

$V = 1296.8 (10) \text{ \AA}^3$

$Z = 4$

$D_x = 1.481 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3626 reflections

$\theta = 2.9\text{--}27.7^\circ$

$\mu = 3.15 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colorless

$0.24 \times 0.20 \times 0.16 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: sealed tube

Monochromator: graphite

$T = 296 \text{ K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{\min} = 0.493$, $T_{\max} = 0.601$

6270 measured reflections

2298 independent reflections

1945 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.106$

$\theta_{\max} = 25.1^\circ$

$\theta_{\min} = 1.6^\circ$

$h = -15 \rightarrow 15$

$k = -9 \rightarrow 8$

$l = -13 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.066$

$wR(F^2) = 0.204$

$S = 1.04$

2298 reflections

155 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

$$w = 1/[\sigma^2(F_o^2) + (0.1306P)^2 + 1.6412P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.84 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.82 \text{ e \AA}^{-3}$

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.77449 (4)	0.08544 (6)	0.80230 (4)	0.0499 (3)
C1	0.3632 (6)	0.5777 (8)	0.3983 (7)	0.0690 (18)
C2	0.4519 (5)	0.6742 (8)	0.4207 (5)	0.0618 (15)
C3	0.5131 (6)	0.7037 (11)	0.3372 (6)	0.084 (2)
H3	0.4949	0.6579	0.2682	0.101*
C4	0.6000 (5)	0.7993 (10)	0.3554 (6)	0.0783 (19)
H4	0.6401	0.8173	0.2986	0.094*
C5	0.6291 (5)	0.8699 (8)	0.4575 (6)	0.0639 (15)
C6	0.5696 (5)	0.8356 (9)	0.5418 (5)	0.0664 (16)
H6	0.5889	0.8784	0.6115	0.080*
C7	0.4814 (5)	0.7378 (8)	0.5231 (6)	0.0672 (16)
H7	0.4425	0.7156	0.5803	0.081*
C8	0.7202 (5)	0.9829 (9)	0.4770 (6)	0.0728 (17)
H8A	0.7083	1.0755	0.4282	0.087*
H8B	0.7251	1.0231	0.5518	0.087*
C9	0.8667 (5)	0.9449 (9)	0.3689 (7)	0.0723 (18)
H9	0.8355	1.0195	0.3182	0.087*
C10	0.9583 (6)	0.8757 (9)	0.3518 (6)	0.0716 (17)
H10	0.9882	0.9006	0.2886	0.086*
C11	1.0081 (5)	0.7671 (7)	0.4288 (6)	0.0644 (16)
C12	0.9567 (5)	0.7273 (8)	0.5214 (7)	0.0741 (19)
H12	0.9871	0.6548	0.5740	0.089*
C13	0.8650 (5)	0.7938 (9)	0.5326 (6)	0.0719 (17)
H13	0.8308	0.7629	0.5918	0.086*
N1	0.2896 (5)	0.4920 (10)	0.3754 (6)	0.0880 (18)
N2	0.8195 (5)	0.9065 (5)	0.4596 (5)	0.0624 (14)
C14	1.0990 (5)	0.6989 (8)	0.4164 (6)	0.0692 (17)
H14A	1.1067	0.5998	0.4581	0.104*
H14B	1.1542	0.7724	0.4422	0.104*
H14C	1.1018	0.6753	0.3402	0.104*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0502 (4)	0.0532 (4)	0.0468 (4)	-0.00751 (19)	0.0074 (3)	-0.00020 (19)
C1	0.056 (4)	0.074 (4)	0.078 (5)	0.005 (3)	0.014 (3)	0.005 (3)
C2	0.057 (3)	0.063 (4)	0.065 (4)	0.009 (3)	0.006 (3)	0.007 (3)
C3	0.083 (5)	0.107 (6)	0.065 (4)	-0.016 (4)	0.019 (4)	-0.004 (4)
C4	0.070 (4)	0.105 (5)	0.064 (4)	-0.013 (4)	0.022 (3)	-0.003 (4)
C5	0.058 (3)	0.060 (3)	0.075 (4)	0.007 (3)	0.012 (3)	0.003 (3)
C6	0.066 (4)	0.075 (4)	0.060 (4)	-0.003 (3)	0.016 (3)	-0.006 (3)
C7	0.067 (4)	0.074 (4)	0.064 (4)	0.003 (3)	0.025 (3)	0.006 (3)

supplementary materials

C8	0.062 (4)	0.069 (4)	0.088 (5)	0.005 (3)	0.016 (3)	-0.002 (4)
C9	0.061 (4)	0.078 (4)	0.078 (5)	-0.002 (3)	0.008 (3)	0.012 (3)
C10	0.066 (4)	0.079 (4)	0.073 (4)	0.003 (3)	0.020 (3)	0.003 (4)
C11	0.051 (3)	0.062 (4)	0.081 (4)	-0.006 (3)	0.010 (3)	-0.002 (3)
C12	0.061 (4)	0.073 (4)	0.088 (5)	0.001 (3)	0.003 (3)	0.010 (4)
C13	0.066 (4)	0.082 (4)	0.071 (4)	-0.002 (3)	0.020 (3)	0.008 (3)
N1	0.062 (3)	0.095 (5)	0.106 (5)	-0.002 (4)	0.011 (3)	-0.002 (4)
N2	0.059 (3)	0.063 (3)	0.066 (4)	0.002 (2)	0.012 (3)	0.006 (2)
C14	0.055 (3)	0.068 (4)	0.086 (5)	0.002 (3)	0.014 (3)	-0.005 (3)

Geometric parameters (Å, °)

C1—N1	1.192 (9)	C8—H8B	0.9700
C1—C2	1.397 (10)	C9—C10	1.355 (10)
C2—C7	1.371 (9)	C9—N2	1.370 (10)
C2—C3	1.390 (10)	C9—H9	0.9300
C3—C4	1.370 (11)	C10—C11	1.399 (10)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.389 (10)	C11—C14	1.330 (9)
C4—H4	0.9300	C11—C12	1.423 (10)
C5—C6	1.392 (9)	C12—C13	1.330 (10)
C5—C8	1.499 (9)	C12—H12	0.9300
C6—C7	1.394 (9)	C13—N2	1.371 (9)
C6—H6	0.9300	C13—H13	0.9300
C7—H7	0.9300	C14—H14A	0.9600
C8—N2	1.471 (8)	C14—H14B	0.9600
C8—H8A	0.9700	C14—H14C	0.9600
N1—C1—C2	177.0 (8)	C10—C9—N2	121.0 (7)
C7—C2—C3	119.1 (6)	C10—C9—H9	119.5
C7—C2—C1	122.0 (6)	N2—C9—H9	119.5
C3—C2—C1	118.9 (7)	C9—C10—C11	120.4 (7)
C4—C3—C2	120.7 (7)	C9—C10—H10	119.8
C4—C3—H3	119.6	C11—C10—H10	119.8
C2—C3—H3	119.6	C14—C11—C10	122.4 (7)
C3—C4—C5	121.0 (6)	C14—C11—C12	120.1 (7)
C3—C4—H4	119.5	C10—C11—C12	117.5 (6)
C5—C4—H4	119.5	C13—C12—C11	119.9 (7)
C4—C5—C6	118.0 (6)	C13—C12—H12	120.0
C4—C5—C8	121.8 (6)	C11—C12—H12	120.0
C6—C5—C8	120.2 (6)	C12—C13—N2	122.0 (7)
C5—C6—C7	120.8 (6)	C12—C13—H13	119.0
C5—C6—H6	119.6	N2—C13—H13	119.0
C7—C6—H6	119.6	C9—N2—C13	119.1 (6)
C2—C7—C6	120.3 (6)	C9—N2—C8	120.3 (6)
C2—C7—H7	119.9	C13—N2—C8	120.6 (6)
C6—C7—H7	119.9	C11—C14—H14A	109.5
N2—C8—C5	113.5 (6)	C11—C14—H14B	109.5
N2—C8—H8A	108.9	H14A—C14—H14B	109.5
C5—C8—H8A	108.9	C11—C14—H14C	109.5

N2—C8—H8B	108.9	H14A—C14—H14C	109.5
C5—C8—H8B	108.9	H14B—C14—H14C	109.5
H8A—C8—H8B	107.7		
C7—C2—C3—C4	-2.2 (12)	N2—C9—C10—C11	-2.0 (11)
C1—C2—C3—C4	179.2 (7)	C9—C10—C11—C14	-178.6 (7)
C2—C3—C4—C5	-0.2 (13)	C9—C10—C11—C12	2.9 (11)
C3—C4—C5—C6	2.4 (11)	C14—C11—C12—C13	-179.0 (7)
C3—C4—C5—C8	-176.3 (7)	C10—C11—C12—C13	-0.5 (11)
C4—C5—C6—C7	-2.1 (10)	C11—C12—C13—N2	-2.9 (11)
C8—C5—C6—C7	176.5 (6)	C10—C9—N2—C13	-1.4 (10)
C3—C2—C7—C6	2.4 (10)	C10—C9—N2—C8	179.9 (7)
C1—C2—C7—C6	-179.0 (6)	C12—C13—N2—C9	3.9 (11)
C5—C6—C7—C2	-0.2 (10)	C12—C13—N2—C8	-177.4 (7)
C4—C5—C8—N2	-61.6 (9)	C5—C8—N2—C9	107.0 (7)
C6—C5—C8—N2	119.8 (7)	C5—C8—N2—C13	-71.7 (8)

Fig. 1

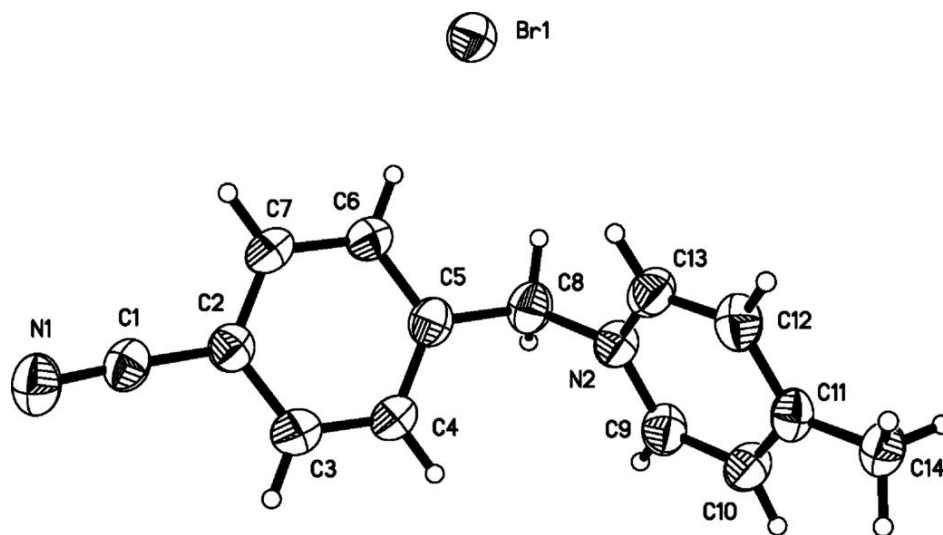


Fig. 2

