

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

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

Hong Chen, Kun Zhu and Guang-Xiang Liu\*

Anhui Key Laboratory of Functional Coordination Compounds, School of Chemistry and Chemical Engineering, Anqing Normal University, Anqing 246003, People's Republic of China

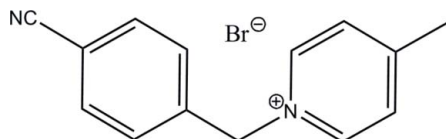
Correspondence e-mail: liugx@live.com

Received 1 May 2009; accepted 26 May 2009

 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  $\Delta$ -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  $\pi$ - $\pi$  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) Å<sup>3</sup>
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 3.15$  mm<sup>-1</sup>  
 $T = 296$  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<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.82$  e Å<sup>-3</sup>

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.

This work was supported by the National Natural Science Foundation of China (No. 20731004), the Natural Science Foundation for Outstanding Scholars of Anhui Province, China (grant No. 044-J-04011) and the Natural Science Foundation of the Education Commission of Anhui Province, China (No. KJ2008B004).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2140).

## References

- Bruker (2000). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.  
 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.

## supporting information

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

**1-(4-Cyanobenzyl)-4-methylpyridinium bromide****Hong Chen, Kun Zhu and Guang-Xiang Liu****S1. Comment**

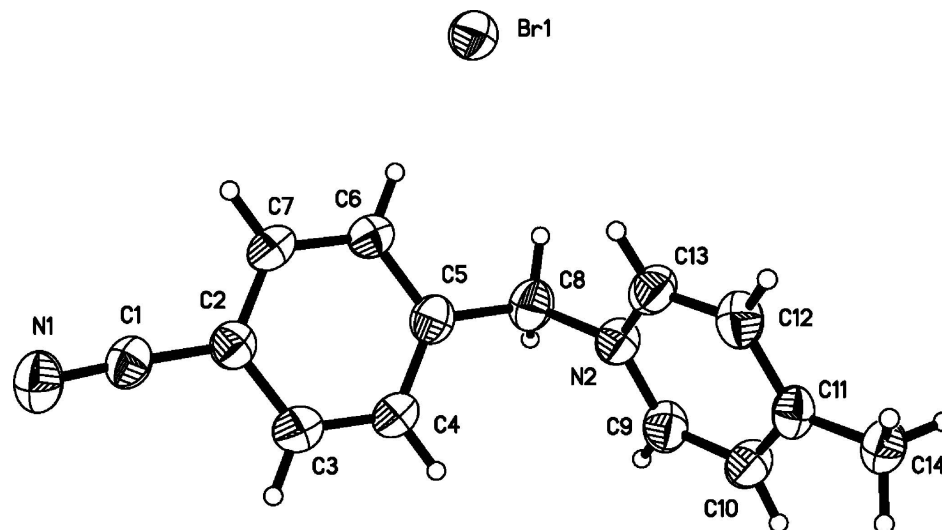
The asymmetric unit of (I) contains one cation and one Br anion (Fig. 1). The cation has a  $\Lambda$ -shaped conformation, and the dihedral angles formed by the C5/C8/N2 plane with the benzene and pyridinium rings are 61.19 (2)° and 72.88 (2)°, respectively (75.8 (2)° between the benzene and pyridinium 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  $\pi$ - $\pi$  interaction between pyridine rings, the distance of centroid-to-centroid is 3.685 Å, which further are linked into one dimensional chain by the  $\pi$ - $\pi$  interaction between benzene ring, the distance of centroid-to-centroid is 4.242 Å. A three-dimensional supramolecular structure was packed *via* Van der Waals forces (Fig. 2).

**S2. Experimental**

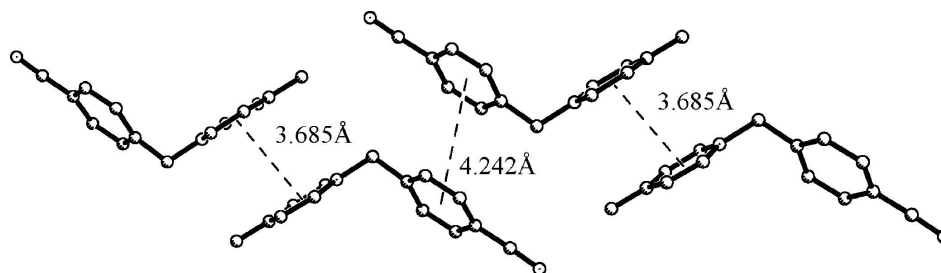
4-cyanobenzyl bromide (10 mmol, 1.96 g) and 4-methylpyridine (20 mmol, 1.88 g) were added to 40 ml of acetone. After stirring and refluxing for 12 h, the mixture was filtered, and the clear solution was allowed to evaporate slowly under inert atmosphere. Block crystals of the title compound were obtained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

**S3. Refinement**

H atoms were positioned geometrically, with C—H = 0.93 Å, 0.96 Å and 0.97 Å 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 Å from atom C16.

**Figure 1**

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

**Figure 2**

One dimensional chain is formed  $\pi$ - $\pi$  interaction along the  $a$ -axis.

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

#### Crystal data

$C_{14}H_{13}N_2^+ \cdot Br^-$   
 $M_r = 289.17$   
 Monoclinic,  $P2_1/c$   
 Hall symbol: -P 2ybc  
 $a = 12.967 (5) \text{ \AA}$   
 $b = 8.217 (4) \text{ \AA}$   
 $c = 12.260 (5) \text{ \AA}$   
 $\beta = 96.900 (5)^\circ$   
 $V = 1296.8 (10) \text{ \AA}^3$   
 $Z = 4$

$F(000) = 584$   
 $D_x = 1.481 \text{ Mg m}^{-3}$   
 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  
 Graphite monochromator  
 $\varphi$  and  $\omega$  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  $I > 2\sigma(I)$

$R_{\text{int}} = 0.106$   
 $\theta_{\text{max}} = 25.1^\circ$ ,  $\theta_{\text{min}} = 1.6^\circ$   
 $h = -15 \rightarrow 15$

$k = -9 \rightarrow 8$   
 $l = -13 \rightarrow 14$

*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  
 0 restraints  
 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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.84 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.82 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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)
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)