Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(1*H*-Tetrazol-5-yl)pyridinium bromide

Wen-Ni Zheng* and Xin-Yuan Chen

Ordered Matter Science Research Center, College of Chemistry and Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China
Correspondence e-mail: fudavid88@yahoo.com.cn

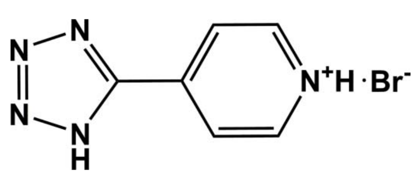
Received 13 November 2010; accepted 3 December 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.029; wR factor = 0.058; data-to-parameter ratio = 17.4.

In the cation of the title compound, $C_6H_6N_5^+\cdot Br^-$, the pyridine and tetrazole rings are nearly coplanar, forming a dihedral angle of 6.41 (2)°. The organic cations interact with the Br^- anions by N—H···Br hydrogen bonds, leading to the formation of chains parallel to the *b* axis.

Related literature

For tetrazole derivatives, see: Zhao *et al.* (2008); Fu *et al.* (2008, 2009). For the crystal structures and properties of related compounds, see: Fu *et al.* (2007, 2009); Fu & Xiong (2008).



Experimental

Crystal data

$C_6H_6N_5^+\cdot Br^-$
M_r = 228.07
Monoclinic, $P2_1$
a = 4.8688 (10) Å
b = 7.6850 (15) Å
c = 11.174 (2) Å
β = 92.38 (3)°
V = 417.73 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.87 mm^{-1}
T = 298 K
0.30 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
4378 measured reflections
1897 independent reflections
1738 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.058
S = 1.08
1897 reflections
109 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 869 Friedel pairs
Flack parameter: 0.045 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Br1^{i}	0.86	2.35	3.210 (3)	178
N2—H2A···Br1^{ii}	0.86	2.37	3.193 (3)	160

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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 a start-up grant from Southeast University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2287).

References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Fu, D.-W., Ge, J.-Z., Dai, J., Ye, H.-Y. & Qu, Z.-R. (2009). *Inorg. Chem. Commun.* **12**, 994–997.
Fu, D.-W., Song, Y.-M., Wang, G.-X., Ye, Q., Xiong, R.-G., Akutagawa, T., Nakamura, T., Chan, P. W. H. & Huang, S.-P. (2007). *J. Am. Chem. Soc.* **129**, 5346–5347.
Fu, D.-W. & Xiong, R.-G. (2008). *Dalton Trans.* pp. 3946–3948.
Fu, D.-W., Zhang, W. & Xiong, R.-G. (2008). *Cryst. Growth Des.* **8**, 3461–3464.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhao, H., Qu, Z.-R., Ye, H.-Y. & Xiong, R.-G. (2008). *Chem. Soc. Rev.* **37**, 84–100.

supplementary materials

Acta Cryst. (2011). E**67**, o53 [**doi:10.1107/S1600536810050658**]

4-(1*H*-Tetrazol-5-yl)pyridinium bromide

W.-N. Zheng and **X.-Y. Chen**

Comment

Tetrazole compounds have attracted attention as phase transition dielectric materials for application in micro-electronics and memory storage. With the purpose of obtaining phase transition crystals of 4-(1*H*-tetrazol-5-yl)pyridine salts, its interaction with various acids has been studied and a series of new materials have been made with this organic molecule (Zhao *et al.*, 2008; Fu *et al.*, 2008; Fu *et al.*, 2007; Fu & Xiong 2008). In this paper, we describe the crystal structure of the title compound, 4-(1*H*-tetrazol-5-yl)pyridinium bromide.

In the title compound (Fig.1), the pyridine N atoms are protonated. The pyridine and tetrazole rings are nearly coplanar and only twisted from each other by a dihedral angle of 6.41 (2)°. The geometric parameters of the tetrazole rings are comparable to those in related molecules (Zhao *et al.*, 2008; Fu *et al.*, 2009).

In the crystal structure, the organic cations are connected by the Br^- anions through two type of N—H···Br hydrogen bonds, with the N···Br distance of 3.210 (3)Å and 3.193 (3) Å, respectively. Those H-bonds link the ionic species into a one-dimensional chain parallel to the *b* axia (Table 1 and Fig.2).

Experimental

Isonicotinonitrile (30 mmol), NaN_3 (45 mmol), NH_4Cl (33 mmol) and DMF (50 ml) were added in a flask under nitrogen atmosphere and the mixture stirred at 110°C for 20 h. The resulting solution was then poured into ice-water (100 ml), and a white solid was obtained after adding HCl (6 *M*) to pH=6. The precipitate was filtered and washed with distilled water. Colourless block-shaped crystals suitable for X-ray analysis were obtained from the crude product by slow evaporation of a water/HBr (50:1 *v*/*v*) solution.

Permittivity measurement show that there is no phase transition within the temperature range (from 100 K to 400 K), and the permittivity is 6.1 at 1 MHz at room temperature.

Refinement

All H atoms attached to C and N atoms were fixed geometrically and treated as riding with C–H = 0.93 Å (aromatic) and N–H = 0.86 Å with U_{iso}(H) =1.2Ueq(C or N).

Figures

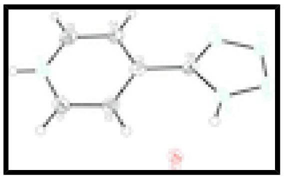


Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

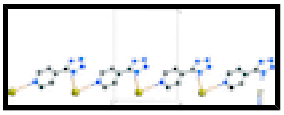


Fig. 2. The crystal packing of the title compound, showing the one-dimensional hydrogen-bonded chain. H atoms not involved in hydrogen bonding (dashed line) have been omitted for clarity.

4-(1*H*-Tetrazol-5-yl)pyridinium bromide

Crystal data

$C_6H_6N_5^+\cdot Br^-$	$F(000) = 224$
$M_r = 228.07$	$D_x = 1.813$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 1897 reflections
$a = 4.8688$ (10) Å	$\theta = 3.2$–27.5°
$b = 7.6850$ (15) Å	$\mu = 4.87$ mm^{-1}
$c = 11.174$ (2) Å	$T = 298$ K
$\beta = 92.38$ (3)°	Block, colorless
$V = 417.73$ (14) Å^3	0.30 × 0.05 × 0.05 mm
$Z = 2$	

Data collection

Rigaku Mercury2 diffractometer	1897 independent reflections
Radiation source: fine-focus sealed tube	1738 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.033$
Detector resolution: 13.66 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
ω scan	$h = -6\rightarrow6$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$k = -9\rightarrow9$
$T_{min} = 0.910$, $T_{max} = 1.000$	$l = -14\rightarrow14$
4378 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.0135P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
1897 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
109 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
1 restraint	Absolute structure: Flack (1983), 869 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.045 (11)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.54779 (5)	0.11064 (8)	0.91219 (2)	0.04195 (11)
C1	0.9198 (7)	0.6502 (5)	0.8550 (3)	0.0389 (10)
H1	1.0123	0.6938	0.9230	0.047*
C2	0.9881 (7)	0.4908 (5)	0.8113 (3)	0.0357 (8)
H2	1.1263	0.4251	0.8494	0.043*
C6	0.9049 (6)	0.2572 (4)	0.6591 (3)	0.0298 (7)
N1	0.7207 (5)	0.7439 (4)	0.8003 (2)	0.0396 (7)
H1A	0.6786	0.8433	0.8297	0.048*
C3	0.8491 (6)	0.4280 (4)	0.7096 (3)	0.0285 (6)
N3	1.0851 (7)	0.0009 (4)	0.6315 (3)	0.0436 (8)
N2	1.1026 (5)	0.1460 (4)	0.6956 (3)	0.0367 (8)
H2A	1.2233	0.1657	0.7524	0.044*
C5	0.5854 (8)	0.6883 (5)	0.7017 (3)	0.0393 (10)
H5	0.4496	0.7575	0.6651	0.047*
N4	0.8778 (6)	0.0253 (4)	0.5546 (3)	0.0424 (8)
C4	0.6457 (7)	0.5292 (5)	0.6541 (3)	0.0355 (9)
H4	0.5513	0.4897	0.5853	0.043*
N5	0.7617 (6)	0.1826 (4)	0.5708 (3)	0.0386 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04736 (18)	0.04135 (19)	0.03641 (18)	0.0106 (2)	−0.00715 (13)	−0.0064 (2)
C1	0.0434 (17)	0.039 (3)	0.0339 (17)	0.0035 (15)	−0.0039 (15)	−0.0041 (15)
C2	0.0334 (18)	0.037 (2)	0.036 (2)	0.0074 (15)	−0.0027 (16)	0.0039 (16)

C6	0.0299 (16)	0.0273 (17)	0.0321 (18)	0.0047 (13)	−0.0010 (14)	0.0065 (14)
N1	0.0515 (17)	0.0286 (15)	0.0393 (16)	0.0081 (13)	0.0075 (15)	−0.0035 (13)
C3	0.0276 (15)	0.0316 (17)	0.0263 (16)	−0.0003 (12)	−0.0003 (13)	0.0061 (13)
N3	0.0523 (19)	0.0330 (18)	0.045 (2)	0.0094 (15)	−0.0047 (17)	−0.0071 (14)
N2	0.0338 (13)	0.038 (3)	0.0371 (14)	0.0048 (13)	−0.0064 (12)	−0.0073 (14)
C5	0.039 (2)	0.037 (2)	0.041 (2)	0.0084 (15)	−0.0007 (18)	0.0101 (17)
N4	0.0475 (19)	0.0360 (18)	0.0431 (19)	0.0054 (16)	−0.0046 (17)	−0.0102 (15)
C4	0.039 (2)	0.0355 (19)	0.032 (2)	0.0060 (15)	−0.0059 (16)	0.0035 (15)
N5	0.0411 (17)	0.0381 (18)	0.0357 (17)	0.0011 (14)	−0.0099 (15)	−0.0036 (13)

Geometric parameters (Å, °)

C1—N1	1.335 (4)	N1—H1A	0.8600
C1—C2	1.365 (5)	C3—C4	1.386 (5)
C1—H1	0.9300	N3—N4	1.312 (5)
C2—C3	1.385 (5)	N3—N2	1.326 (4)
C2—H2	0.9300	N2—H2A	0.8600
C6—N5	1.315 (4)	C5—C4	1.370 (4)
C6—N2	1.338 (4)	C5—H5	0.9300
C6—C3	1.459 (4)	N4—N5	1.350 (3)
N1—C5	1.330 (5)	C4—H4	0.9300
N1—C1—C2	120.2 (3)	C4—C3—C6	118.2 (3)
N1—C1—H1	119.9	N4—N3—N2	105.3 (3)
C2—C1—H1	119.9	N3—N2—C6	110.1 (3)
C1—C2—C3	119.2 (3)	N3—N2—H2A	125.0
C1—C2—H2	120.4	C6—N2—H2A	125.0
C3—C2—H2	120.4	N1—C5—C4	120.1 (4)
N5—C6—N2	107.6 (3)	N1—C5—H5	120.0
N5—C6—C3	125.5 (3)	C4—C5—H5	120.0
N2—C6—C3	126.8 (3)	N3—N4—N5	110.8 (3)
C5—N1—C1	122.1 (3)	C5—C4—C3	119.2 (4)
C5—N1—H1A	119.0	C5—C4—H4	120.4
C1—N1—H1A	119.0	C3—C4—H4	120.4
C2—C3—C4	119.2 (3)	C6—N5—N4	106.2 (3)
C2—C3—C6	122.6 (3)		
N1—C1—C2—C3	0.2 (5)	C3—C6—N2—N3	177.7 (3)
C2—C1—N1—C5	−1.0 (6)	C1—N1—C5—C4	1.0 (5)
C1—C2—C3—C4	0.5 (5)	N2—N3—N4—N5	−1.1 (4)
C1—C2—C3—C6	−178.4 (3)	N1—C5—C4—C3	−0.2 (5)
N5—C6—C3—C2	172.4 (3)	C2—C3—C4—C5	−0.6 (5)
N2—C6—C3—C2	−5.2 (5)	C6—C3—C4—C5	178.4 (3)
N5—C6—C3—C4	−6.6 (5)	N2—C6—N5—N4	−0.4 (4)
N2—C6—C3—C4	175.8 (3)	C3—C6—N5—N4	−178.4 (3)
N4—N3—N2—C6	0.8 (4)	N3—N4—N5—C6	1.0 (4)
N5—C6—N2—N3	−0.3 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N1—H1A···Br1^{i}	0.86	2.35	3.210 (3)	178
N2—H2A···Br1^{ii}	0.86	2.37	3.193 (3)	160

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

Fig. 1

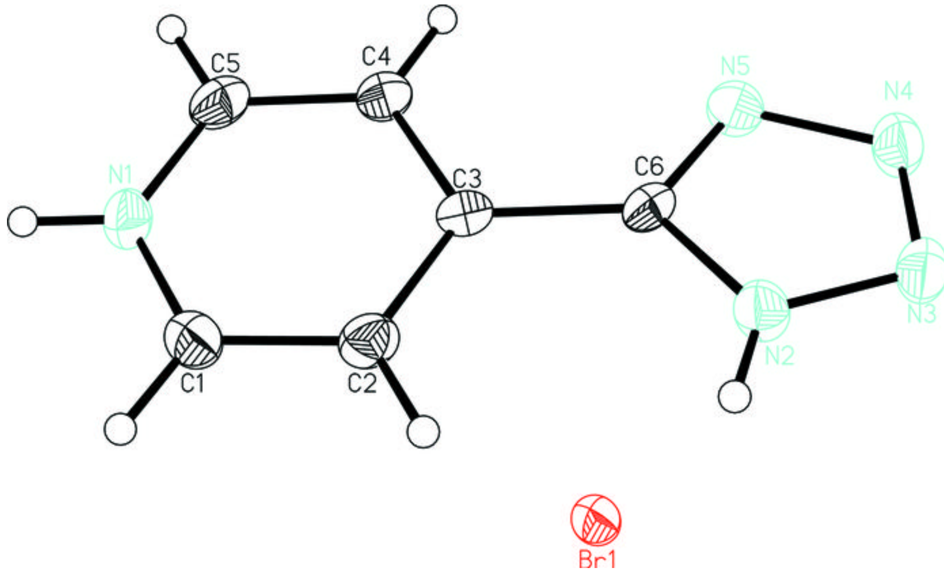


Fig. 2