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## Structure Reports

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

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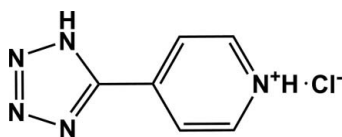
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 Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.071; data-to-parameter ratio = 16.7.

In the cation of the title compound,  $\text{C}_6\text{H}_6\text{N}_5^+\cdot\text{Cl}^-$ , the tetrazole and pyridine rings are nearly coplanar, making a dihedral angle of  $5.58(11)^\circ$ . The organic cations are linked to the chloride anions *via*  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds, forming chains along [110].

## Related literature

For supramolecular self-assembly chemistry, see: Fender *et al.* (2002). For the structures of related tetrazole derivatives, see: Fu *et al.* (2009).



## Experimental

## Crystal data

$\text{C}_6\text{H}_6\text{N}_5^+\cdot\text{Cl}^-$   
 $M_r = 183.61$   
 Monoclinic,  $P2_1$   
 $a = 4.8552(10)$  Å  
 $b = 7.5862(15)$  Å  
 $c = 10.884(2)$  Å  
 $\beta = 92.88(3)^\circ$

$V = 400.36(14)$  Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.42$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.30 \times 0.05 \times 0.05$  mm

## Data collection

Rigaku Mercury CCD diffractometer  
 Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)  
 $T_{\min} = 0.910$ ,  $T_{\max} = 1.000$

4104 measured reflections  
 1825 independent reflections  
 1687 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.071$   
 $S = 1.11$   
 1825 reflections  
 109 parameters  
 1 restraint

H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.26$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 840 Friedel pairs  
 Flack parameter: 0.07 (6)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{Cl1}^{\text{i}}$	0.86	2.21	3.0704 (18)	176
$\text{N5}-\text{H5A}\cdots\text{Cl1}^{\text{ii}}$	0.86	2.22	3.0344 (18)	159

 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: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by a start-up grant from Anyang Institute of Technology, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5091).

## References

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# supporting information

*Acta Cryst.* (2010). E66, o3297 [https://doi.org/10.1107/S1600536810047756]

## 4-(1*H*-Tetrazol-5-yl)pyridinium chloride

**Yan-Wei Zhang**

### S1. Comment

In recent years there is a rapidly increasing interest in the construction of various kinds of supramolecular systems for understanding molecular self-assembly principles and for designing molecular recognition devices (Fender *et al.* 2002). We report here the crystal structure of the title compound, 4-(1*H*-tetrazol-5-yl)pyridinium chloride.

In the title compound (Fig.1), the pyridine N atom is protonated. The tetrazole and pyridine rings are nearly coplanar and only twisted from each other by a dihedral angle of 5.58 (11)°. The geometric parameters of the tetrazole rings are comparable to those in related molecules (Fu *et al.*, 2009).

In the crystal structure, the organic cations are connected by the Cl<sup>-</sup> anions through two type of N—H···Cl hydrogen bonds, with the N···Cl distance of 3.0704 (2) Å and 3.0344 (2) Å, respectively. Those H-bonds link the ion units into a one-dimensional chain along the [1 1 0] direction (Table 1 and Fig. 2).

### S2. Experimental

4-(1*H*-Tetrazol-5-yl)pyridinium chloride was obtained commercially, and the single crystals were obtained from an ethanol solution.

### S3. Refinement

H atoms attached to N atoms were located in a difference Fourier map, and refined in riding mode with N—H = 0.86 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ . Other H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

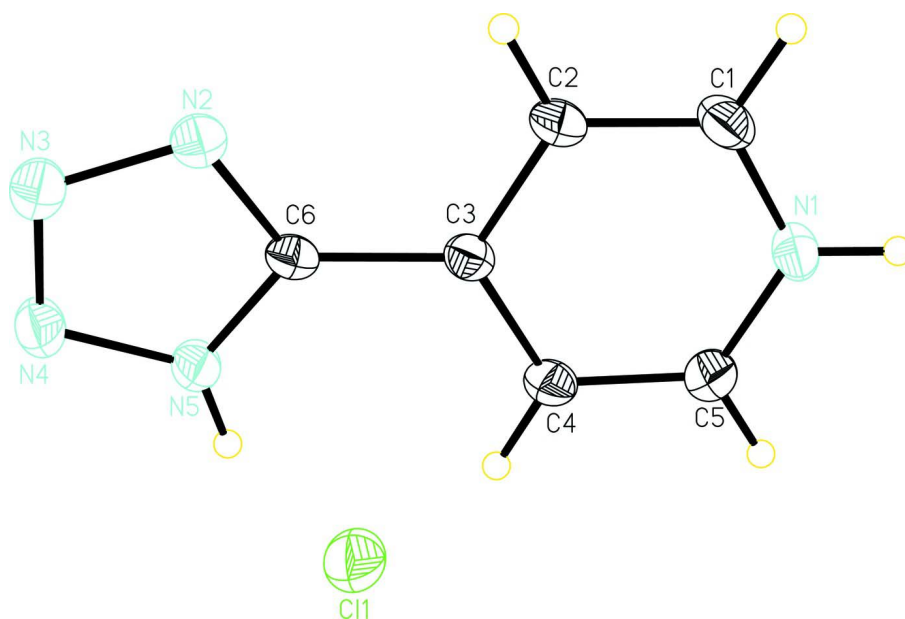


Figure 1

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

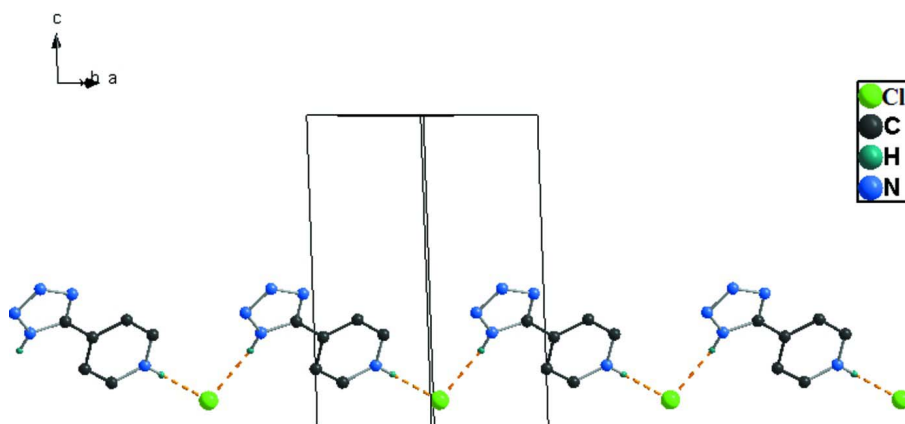


Figure 2

Part of the crystal packing of the title compound. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

#### 4-(1*H*-Tetrazol-5-yl)pyridinium chloride

##### Crystal data

$C_6H_6N_5^+ \cdot Cl^-$

$M_r = 183.61$

Monoclinic,  $P2_1$

Hall symbol: P 2yb

$a = 4.8552 (10) \text{ \AA}$

$b = 7.5862 (15) \text{ \AA}$

$c = 10.884 (2) \text{ \AA}$

$\beta = 92.88 (3)^\circ$

$V = 400.36 (14) \text{ \AA}^3$

$Z = 2$

$F(000) = 188$   
 $D_x = 1.523 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 1825 reflections  
 $\theta = 3.3\text{--}27.5^\circ$

$\mu = 0.42 \text{ mm}^{-1}$   
 $T = 298 \text{ K}$   
 Block, colorless  
 $0.30 \times 0.05 \times 0.05 \text{ mm}$

*Data collection*

Rigaku Mercury CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution: 13.6612 pixels  $\text{mm}^{-1}$   
 $\varphi$  and  $\omega$  scan  
 Absorption correction: multi-scan  
 (*CrystalClear*; Rigaku, 2005)  
 $T_{\min} = 0.910$ ,  $T_{\max} = 1.000$

4104 measured reflections  
 1825 independent reflections  
 1687 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$   
 $\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.3^\circ$   
 $h = -6 \rightarrow 6$   
 $k = -9 \rightarrow 9$   
 $l = -14 \rightarrow 14$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.071$   
 $S = 1.11$   
 1825 reflections  
 109 parameters  
 1 restraint  
 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  
 $w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 0.0441P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e \AA}^{-3}$   
 Absolute structure: Flack (1983), 840 Friedel  
 pairs  
 Absolute structure parameter: 0.07 (6)

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
N3	0.6191 (4)	0.2346 (2)	0.94401 (17)	0.0448 (5)
C4	0.5024 (4)	0.7071 (3)	0.67942 (18)	0.0354 (4)
H4	0.3611	0.6417	0.6407	0.043*
N4	0.4093 (4)	0.2114 (2)	0.86534 (18)	0.0426 (4)
N5	0.3900 (3)	0.3586 (2)	0.79785 (15)	0.0356 (4)
H5A	0.2678	0.3786	0.7396	0.043*
C6	0.5897 (4)	0.4690 (2)	0.83517 (16)	0.0290 (4)
N1	0.7754 (3)	0.9626 (2)	0.69060 (16)	0.0390 (4)
H1A	0.8175	1.0632	0.6604	0.047*

C2	0.8551 (4)	0.7442 (3)	0.83953 (19)	0.0360 (5)
H2	0.9528	0.7030	0.9094	0.043*
N2	0.7348 (4)	0.3944 (2)	0.92686 (16)	0.0389 (4)
C1	0.9159 (5)	0.9050 (3)	0.7917 (2)	0.0400 (5)
H1	1.0541	0.9743	0.8292	0.048*
C5	0.5724 (4)	0.8690 (3)	0.63512 (18)	0.0401 (5)
H5	0.4775	0.9142	0.5657	0.048*
C3	0.6467 (4)	0.6419 (3)	0.78358 (16)	0.0293 (4)
Cl1	0.95294 (9)	0.32109 (6)	0.59025 (4)	0.04239 (15)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N3	0.0493 (10)	0.0393 (10)	0.0450 (10)	−0.0036 (9)	−0.0050 (8)	0.0062 (9)
C4	0.0335 (10)	0.0399 (11)	0.0322 (10)	−0.0090 (9)	−0.0049 (8)	−0.0024 (8)
N4	0.0449 (10)	0.0337 (10)	0.0484 (10)	−0.0080 (8)	−0.0059 (8)	0.0056 (8)
N5	0.0347 (8)	0.0346 (11)	0.0366 (8)	−0.0080 (7)	−0.0062 (7)	0.0042 (7)
C6	0.0258 (9)	0.0326 (10)	0.0286 (8)	−0.0027 (7)	−0.0009 (7)	−0.0047 (7)
N1	0.0460 (10)	0.0302 (9)	0.0412 (9)	−0.0088 (8)	0.0058 (8)	0.0008 (7)
C2	0.0338 (10)	0.0387 (11)	0.0345 (10)	−0.0071 (9)	−0.0083 (8)	−0.0026 (9)
N2	0.0416 (9)	0.0362 (9)	0.0377 (9)	−0.0024 (8)	−0.0082 (7)	0.0023 (7)
C1	0.0381 (11)	0.0380 (11)	0.0436 (12)	−0.0112 (9)	−0.0019 (9)	−0.0067 (10)
C5	0.0442 (11)	0.0419 (13)	0.0338 (10)	−0.0059 (9)	−0.0021 (9)	0.0036 (8)
C3	0.0296 (9)	0.0299 (9)	0.0285 (9)	−0.0029 (7)	0.0028 (7)	−0.0042 (7)
Cl1	0.0465 (3)	0.0433 (3)	0.0362 (2)	−0.0112 (3)	−0.00936 (18)	0.0070 (2)

*Geometric parameters (Å, °)*

N3—N4	1.309 (3)	C6—C3	1.459 (3)
N3—N2	1.353 (2)	N1—C5	1.334 (3)
C4—C5	1.369 (3)	N1—C1	1.338 (3)
C4—C3	1.393 (3)	N1—H1A	0.8600
C4—H4	0.9300	C2—C1	1.365 (3)
N4—N5	1.337 (2)	C2—C3	1.391 (3)
N5—C6	1.330 (2)	C2—H2	0.9300
N5—H5A	0.8600	C1—H1	0.9300
C6—N2	1.320 (2)	C5—H5	0.9300
N4—N3—N2	110.18 (18)	C1—C2—C3	119.9 (2)
C5—C4—C3	118.78 (19)	C1—C2—H2	120.0
C5—C4—H4	120.6	C3—C2—H2	120.0
C3—C4—H4	120.6	C6—N2—N3	106.21 (16)
N3—N4—N5	106.13 (17)	N1—C1—C2	119.6 (2)
C6—N5—N4	109.17 (15)	N1—C1—H1	120.2
C6—N5—H5A	125.4	C2—C1—H1	120.2
N4—N5—H5A	125.4	N1—C5—C4	120.6 (2)
N2—C6—N5	108.31 (17)	N1—C5—H5	119.7
N2—C6—C3	124.90 (17)	C4—C5—H5	119.7

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N5—C6—C3	126.77 (16)	C2—C3—C4	118.91 (18)
C5—N1—C1	122.22 (18)	C2—C3—C6	118.76 (17)
C5—N1—H1A	118.9	C4—C3—C6	122.33 (17)
C1—N1—H1A	118.9		

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*Hydrogen-bond geometry (Å, °)*

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<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1A $\cdots$ C11 <sup>i</sup>	0.86	2.21	3.0704 (18)	176
N5—H5A $\cdots$ C11 <sup>ii</sup>	0.86	2.22	3.0344 (18)	159

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