Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Yan-Wei Zhang

Department of Chemical & Environmental Engineering, Anyang Institute of Technology, Anyang 455000, People's Republic of China
Correspondence e-mail: ayitzhang@yahoo.com.cn

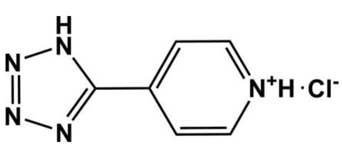
Received 16 November 2010; accepted 17 November 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–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, $C_6H_6N_5^+\cdot Cl^-$, the tetrazole and pyridine rings are nearly coplanar, making a dihedral angle of 5.58 (11)°. The organic cations are linked to the chloride anions *via* N—H⋯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

$C_6H_6N_5^+\cdot Cl^-$
M_r = 183.61
Monoclinic, $P2_1$
a = 4.8552 (10) Å
b = 7.5862 (15) Å
c = 10.884 (2) Å
β = 92.88 (3)°
V = 400.36 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 298 K
0.30 × 0.05 × 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_{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^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 840 Friedel pairs
Flack parameter: 0.07 (6)

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*A*⋯Cl1^{i}	0.86	2.21	3.0704 (18)	176
N5—H5*A*⋯Cl1^{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

Fender, N. S., Kahwa, I. A. & Fronczek, F. R. (2002). *J. Solid State Chem.* **163**, 286–293.
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.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, o3297 [doi:10.1107/S1600536810047756]

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

Y.-W. Zhang

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^- 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).

Experimental

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

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_{iso}(H) = $1.2U_{eq}$(N). Other H atoms were fixed geometrically and treated as riding with C–H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C).

Figures

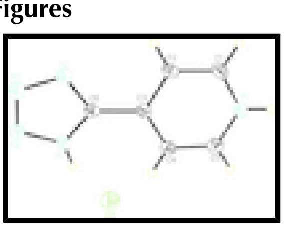


Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

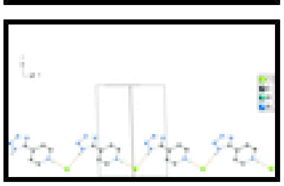


Fig. 2. Part of the crystal packing of the title compound. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

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

Crystal data

$C_6H_6N_5^+\cdot Cl^-$	$F(000) = 188$
$M_r = 183.61$	$D_x = 1.523$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 1825 reflections
$a = 4.8552$ (10) Å	$\theta = 3.3–27.5°$
$b = 7.5862$ (15) Å	$\mu = 0.42$ mm^{-1}
$c = 10.884$ (2) Å	$T = 298$ K
$\beta = 92.88$ (3)°	Block, colorless
$V = 400.36$ (14) Å^3	0.30 × 0.05 × 0.05 mm
$Z = 2$	

Data collection

Rigaku Mercury CCD diffractometer	1825 independent reflections
Radiation source: fine-focus sealed tube	1687 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.024$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
φ and ω scan	$h = -6\rightarrow6$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$k = -9\rightarrow9$
$T_{min} = 0.910$, $T_{max} = 1.000$	$l = -14\rightarrow14$
4104 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
$R[F^2 > 2\sigma(F^2)] = 0.031$	H-atom parameters constrained
$wR(F^2) = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 0.0441P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} < 0.001$
1825 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
109 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
1 restraint	Absolute structure: Flack (1983), 840 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack 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 (Å^2)

	x	y	z	U_{iso}*/U_{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^2)

	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
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		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···Cl1^{i}	0.86	2.21	3.0704 (18)	176
N5—H5A···Cl1^{ii}	0.86	2.22	3.0344 (18)	159

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

Fig. 1

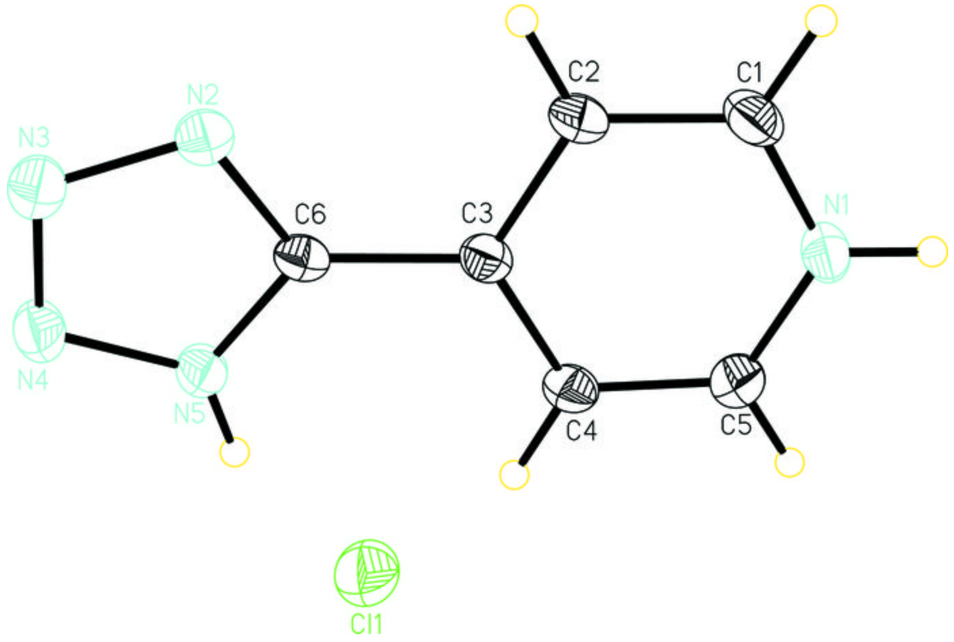


Fig. 2