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5-(Pyridinium-4-yl)-1*H*-1,2,3,4-tetrazol-1-ide

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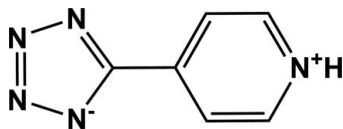
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å;
 R factor = 0.040; wR factor = 0.096; data-to-parameter ratio = 7.2.

In the title zwitterionic molecule, $\text{C}_6\text{H}_5\text{N}_5$, the tetrazole and pyridine rings are nearly coplanar, making a dihedral angle of 2.08 (1)°. In the crystal, molecules are connected by classical $\text{N}-\text{H}\cdots\text{N}$ and weak $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds.

Related literature

For applications of 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

$\text{C}_6\text{H}_5\text{N}_5$
 $M_r = 147.15$
Monoclinic, Cc
 $a = 7.0508$ (14) Å
 $b = 7.4007$ (15) Å
 $c = 11.926$ (2) Å
 $\beta = 96.56$ (3)°

$V = 618.2$ (2) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 298$ K
 $0.30 \times 0.20 \times 0.15$ mm

Data collection

Rigaku Mercury2 diffractometer
3122 measured reflections
719 independent reflections

633 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.096$
 $S = 1.13$
719 reflections
100 parameters

2 restraints
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{N2}^{\text{i}}$	0.86	1.89	2.745 (4)	176
$\text{N1}-\text{H1A}\cdots\text{N3}^{\text{i}}$	0.86	2.52	3.306 (4)	152
$\text{C1}-\text{H1}\cdots\text{N5}^{\text{ii}}$	0.93	2.46	3.308 (4)	152
$\text{C5}-\text{H5}\cdots\text{N4}^{\text{iii}}$	0.93	2.38	3.168 (4)	142

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x, y + 1, z$; (iii) $x + \frac{1}{2}, -y - \frac{1}{2}, z + \frac{1}{2}$.

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5093).

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supplementary materials

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5-(Pyridinium-4-yl)-1*H*-1,2,3,4-tetrazol-1-ide

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Comment

Tetrazole compounds attracted more attention as phase transition dielectric materials for its application in micro-electronics, memory storage. With the purpose of obtaining phase transition crystals of tetrazole compound, a series of new materials have been elaborated with this organic molecule (Zhao *et al.*, 2008; Fu *et al.*, 2008; Fu *et al.*, 2007; Fu & Xiong 2008). We report here the crystal structure of the title compound, 5-(pyridinium-4-yl)tetrazol-1-ide.

The dielectric constant of title compound as a function of temperature indicates that the permittivity is basically temperature-independent, suggesting that this compound should be not a real ferroelectrics or there may be no distinct phase transition occurred within the measured temperature range. Similarly, below the melting point (413K) of the compound, the dielectric constant as a function of temperature also goes smoothly, and there is no dielectric anomaly observed (dielectric constant equaling to 6.1 to 7.9).

In the title compound (Fig.1), the pyridine N atom is protonated, thus indicating a positive charge in the pyridine N atom. And the tetrazole ring was showing a negative charge to make the charge balance. The tetrazole and pyridine rings are twisted from each other by a dihedral angle of 2.08 (1)°. The geometric parameters of the tetrazole rings are comparable to those in related molecules (Fu *et al.*, 2009).

In the crystal structure the molecules are connected by classic N—H···N and weak C—H···N hydrogen bonds (Table 1).

Experimental

5-(Pyridinium-4-yl)tetrazol-1-ide 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 $U_{iso}(H) = 1.2U_{eq}(C)$. As no significant anomalous scattering, Friedel pairs were merged.

Figures

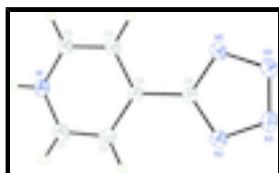


Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

5-(Pyridinium-4-yl)-1H-1,2,3,4-tetrazol-1-ide

Crystal data

$C_6H_5N_5$	$F(000) = 304$
$M_r = 147.15$	$D_x = 1.581 \text{ Mg m}^{-3}$
Monoclinic, Cc	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: C -2yc	Cell parameters from 1425 reflections
$a = 7.0508 (14) \text{ \AA}$	$\theta = 3.4\text{--}24.5^\circ$
$b = 7.4007 (15) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 11.926 (2) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 96.56 (3)^\circ$	Block, colorless
$V = 618.2 (2) \text{ \AA}^3$	$0.30 \times 0.20 \times 0.15 \text{ mm}$
$Z = 4$	

Data collection

Rigaku Mercury2 diffractometer	633 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube graphite	$R_{\text{int}} = 0.039$
Detector resolution: $13.6612 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.4^\circ$
CCD profile fitting scans	$h = -9 \rightarrow 9$
3122 measured reflections	$k = -9 \rightarrow 9$
719 independent reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.096$	H-atom parameters constrained
$S = 1.13$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2]$
719 reflections	where $P = (F_o^2 + 2F_c^2)/3$
100 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
2 restraints	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	1.0961 (4)	0.3035 (4)	0.4442 (2)	0.0382 (6)
H1A	1.1462	0.3791	0.4937	0.046*
N2	0.7525 (4)	-0.0341 (4)	0.1099 (2)	0.0375 (6)
N3	0.7094 (4)	-0.1968 (3)	0.0653 (2)	0.0443 (7)
N4	0.7884 (4)	-0.3224 (3)	0.1321 (2)	0.0444 (8)
N5	0.8864 (3)	-0.2457 (4)	0.2218 (2)	0.0395 (7)
C1	0.9963 (5)	0.3659 (4)	0.3504 (3)	0.0397 (9)
H1	0.9805	0.4896	0.3394	0.048*
C2	0.9185 (4)	0.2487 (4)	0.2718 (3)	0.0368 (7)
H2	0.8496	0.2920	0.2062	0.044*
C3	0.9406 (4)	0.0634 (4)	0.2879 (2)	0.0290 (6)
C4	1.0442 (4)	0.0050 (4)	0.3861 (2)	0.0372 (8)
H4	1.0622	-0.1179	0.3996	0.045*
C5	1.1202 (4)	0.1280 (4)	0.4632 (3)	0.0391 (7)
H5	1.1896	0.0888	0.5298	0.047*
C6	0.8605 (4)	-0.0704 (4)	0.2067 (2)	0.0305 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0486 (14)	0.0342 (16)	0.0299 (14)	-0.0035 (13)	-0.0037 (10)	-0.0059 (13)
N2	0.0465 (15)	0.0288 (12)	0.0353 (13)	0.0003 (11)	-0.0040 (10)	0.0010 (11)
N3	0.0595 (17)	0.0348 (13)	0.0359 (13)	-0.0060 (15)	-0.0060 (11)	-0.0082 (14)
N4	0.062 (2)	0.0293 (14)	0.0404 (19)	-0.0004 (13)	-0.0010 (15)	-0.0045 (12)
N5	0.0533 (16)	0.0251 (13)	0.0377 (16)	0.0014 (11)	-0.0051 (13)	-0.0026 (11)
C1	0.0455 (17)	0.029 (2)	0.0431 (16)	0.0041 (15)	0.0005 (13)	0.0020 (15)
C2	0.0422 (17)	0.0311 (16)	0.0346 (16)	0.0031 (13)	-0.0059 (12)	0.0052 (13)
C3	0.0355 (14)	0.0240 (15)	0.0264 (13)	0.0001 (12)	-0.0007 (11)	-0.0009 (11)
C4	0.0514 (19)	0.0257 (18)	0.0319 (15)	0.0008 (12)	-0.0060 (12)	-0.0004 (13)
C5	0.0512 (18)	0.0331 (16)	0.0304 (14)	0.0035 (14)	-0.0069 (13)	-0.0014 (13)
C6	0.0369 (16)	0.0263 (15)	0.0272 (14)	0.0002 (12)	-0.0016 (11)	0.0014 (13)

Geometric parameters (\AA , $^\circ$)

N1—C5	1.325 (4)	C1—H1	0.9300
N1—C1	1.334 (5)	C2—C3	1.391 (4)
N1—H1A	0.8600	C2—H2	0.9300
N2—C6	1.335 (4)	C3—C4	1.377 (4)
N2—N3	1.337 (4)	C3—C6	1.453 (4)
N3—N4	1.306 (4)	C4—C5	1.359 (4)

supplementary materials

N4—N5	1.333 (4)	C4—H4	0.9300
N5—C6	1.320 (4)	C5—H5	0.9300
C1—C2	1.348 (5)		
C5—N1—C1	121.8 (3)	C4—C3—C2	117.8 (3)
C5—N1—H1A	119.1	C4—C3—C6	118.8 (2)
C1—N1—H1A	119.1	C2—C3—C6	123.4 (2)
C6—N2—N3	104.1 (3)	C5—C4—C3	119.6 (3)
N4—N3—N2	109.6 (3)	C5—C4—H4	120.2
N3—N4—N5	109.4 (2)	C3—C4—H4	120.2
C6—N5—N4	104.9 (2)	N1—C5—C4	120.5 (3)
N1—C1—C2	119.6 (3)	N1—C5—H5	119.7
N1—C1—H1	120.2	C4—C5—H5	119.7
C2—C1—H1	120.2	N5—C6—N2	111.8 (3)
C1—C2—C3	120.5 (3)	N5—C6—C3	122.8 (2)
C1—C2—H2	119.7	N2—C6—C3	125.4 (3)
C3—C2—H2	119.7		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots N2 ⁱ	0.86	1.89	2.745 (4)	176
N1—H1A \cdots N3 ⁱ	0.86	2.52	3.306 (4)	152
C1—H1 \cdots N5 ⁱⁱ	0.93	2.46	3.308 (4)	152
C5—H5 \cdots N4 ⁱⁱⁱ	0.93	2.38	3.168 (4)	142

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $x, y+1, z$; (iii) $x+1/2, -y-1/2, z+1/2$.

Fig. 1

