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4-Cyanopyridinium chloride

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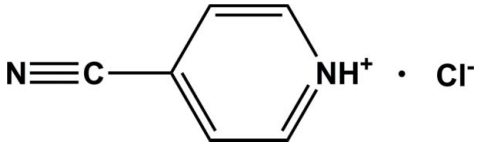
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.008 Å; R factor = 0.086; wR factor = 0.234; data-to-parameter ratio = 15.0.

In the crystal structure of the title salt, $C_6H_5N_2^+\cdot Cl^-$, the pyridinium cation links to the Cl^- anion *via* an N—H···Cl hydrogen bond. Weak C—H···Cl interactions also occur.

Related literature

For the structures and properties of related compounds, see: Chen *et al.* (2000); Dai & Chen (2011); Xu *et al.* (2011); Liu *et al.* (1999); Zhao *et al.* (2003); Zheng (2011).



Experimental

Crystal data

$C_6H_5N_2^+\cdot Cl^-$
M_r = 140.57
Triclinic, $P\overline{1}$
a = 6.6166 (2) Å
b = 7.6552 (3) Å
c = 8.3495 (5) Å
α = 63.957 (5)°
β = 69.830 (2)°
γ = 74.367 (4)°
V = 353.16 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 123 K
0.10 × 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
3077 measured reflections
1231 independent reflections
1078 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.234
S = 1.32
1231 reflections
82 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1^{i}	0.90	2.14	3.033 (5)	174
C4—H4A···Cl1	0.95	2.71	3.566 (5)	151
C5—H5A···Cl1^{ii}	0.95	2.65	3.566 (6)	161

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

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: XU5524).

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supplementary materials

Acta Cryst. (2012). E**68**, o1611 [doi:10.1107/S1600536812018648]

4-Cyanopyridinium chloride

Wen-Ni Zheng

Comment

Simple organic salts containing strong intrermolecular H-bonds have attracted an attention as materials which display ferroelectric-paraelectric phase transitions (Chen *et al.*, 2000; Liu *et al.*, 1999; Zhao *et al.*, 2003). With the purpose of obtaining phase transition crystals of organic salts, various organic molecules have been studied and a series of new materials have been elaborated (Dai & Chen, 2011; Xu *et al.*, 2011; Zheng, 2011). Herewith we present the synthesis and crystal structure of the title compound.

In the title compound (Fig. 1), the bond lengths and angles have normal values. The asymmetric unit was composed of one 4-cyanopyridinium cation and one Cl^- anion. The protonated N atom was involved in strong intramolecular N—H···Cl hydrogen bonds with the N···Cl distance of 3.033 (5)Å. The weak intermolecular C4—H4A···Cl1 and C5—H45···Cl1 interactions were presented in the crystal structure with C5···Cl1 = 3.566 (5)Å and C5···Cl1 = 3.566 (6)Å, respectively. The crystal packing is further stabilized by aromatic $\pi\cdots\pi$ interactions between the pyridine rings of the neighbouring 4-cyanopyridinium cations with the Cg···Cg distances of 4.416 (5) Å and 4.102 (5) Å (Cg is the centroide of the pyridine ring) (Fig. 2 and Table 1).

Experimental

The HCl (5 mL), isonicotinonitrile (20 mmol) and ethanol (50 mL) were added into a 100 mL flask. The mixture was stirred at 333 K for 2 h, and then the precipitate was filtrated out. Colourless crystals suitable for X-ray diffraction were obtained by slow evaporation of the solution.

Refinement

All the H atoms were situated into the idealized positions and treated as riding with C–H = 0.95 and N—H = 0.90 Å, U_{iso}(H) = 1.2U_{eq}(C,N).

Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

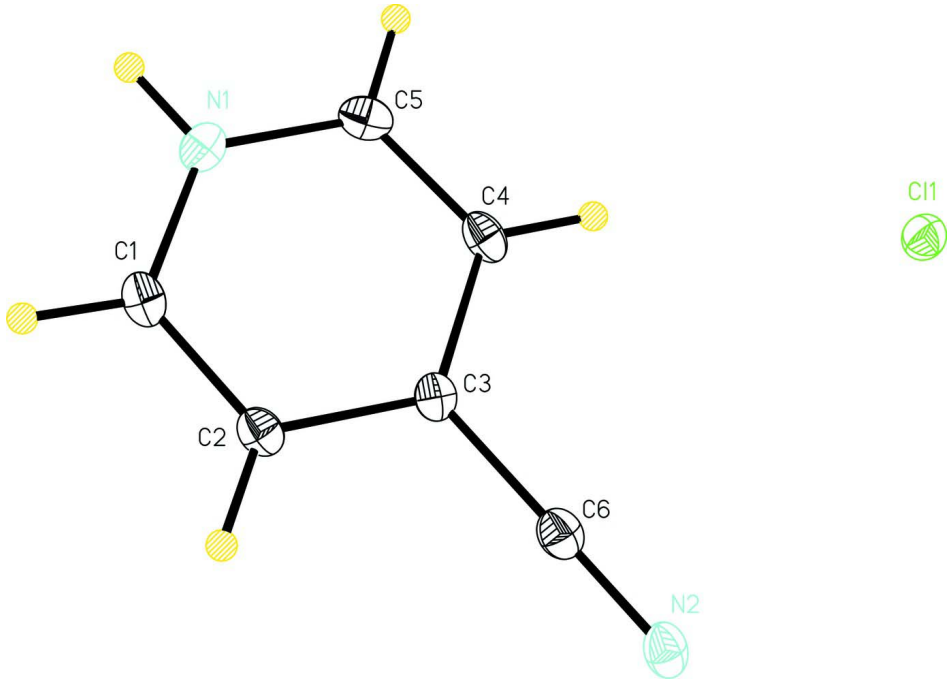

Figure 1

A view of the asymmetric unit with the atomic numbering scheme. The displacement ellipsoids were drawn at the 30% probability level.

4-Cyanopyridinium chloride

Crystal data

$C_6H_5N_2^+\cdot Cl^-$
$M_r = 140.57$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.6166\ (2)$ Å
$b = 7.6552\ (3)$ Å
$c = 8.3495\ (5)$ Å
$\alpha = 63.957\ (5)°$
$\beta = 69.830\ (2)°$
$\gamma = 74.367\ (4)°$
$V = 353.16\ (3)$ Å^3
$Z = 2$
$F(000) = 144$
$D_x = 1.322$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1231 reflections
$\theta = 2.8–27.5°$
$\mu = 0.45$ mm^{-1}
$T = 123$ K
Block, colorless
0.10 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.910$, $T_{max} = 1.000$
3077 measured reflections
1231 independent reflections
1078 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -7\rightarrow7$
$k = -9\rightarrow9$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.086$
$wR(F^2) = 0.234$
$S = 1.32$
1231 reflections
82 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
$w = 1/[\sigma^2(F_o^2) + (0.0002P)^2 + 3.2997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.97$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N2	0.8017 (7)	0.1582 (6)	0.6278 (6)	0.0267 (11)
N1	0.4202 (7)	0.2736 (6)	0.0960 (6)	0.0234 (10)
H1	0.3576	0.2900	0.0094	0.028*
C1	0.6318 (8)	0.1817 (7)	0.0856 (7)	0.0238 (12)
H1A	0.7092	0.1377	−0.0122	0.029*
C3	0.6118 (8)	0.2221 (7)	0.3646 (6)	0.0192 (11)
C4	0.3919 (8)	0.3182 (7)	0.3713 (7)	0.0238 (13)
H4A	0.3103	0.3648	0.4667	0.029*
C6	0.7156 (8)	0.1908 (7)	0.5071 (7)	0.0258 (13)
C5	0.3016 (8)	0.3411 (7)	0.2334 (7)	0.0251 (13)
H5A	0.1565	0.4042	0.2349	0.030*
C2	0.7328 (8)	0.1531 (7)	0.2198 (7)	0.0222 (12)
H2A	0.8783	0.0894	0.2146	0.027*
Cl1	0.1808 (2)	0.31778 (18)	0.82634 (17)	0.0249 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.031 (2)	0.021 (2)	0.0189 (19)	−0.0006 (18)	−0.0026 (17)	−0.0048 (16)
N1	0.031 (2)	0.0187 (18)	0.0204 (18)	−0.0053 (17)	−0.0098 (16)	−0.0034 (15)
C1	0.028 (2)	0.017 (2)	0.020 (2)	−0.001 (2)	−0.0027 (19)	−0.0056 (18)
C3	0.024 (2)	0.0126 (19)	0.015 (2)	−0.0054 (18)	−0.0029 (18)	−0.0008 (16)
C4	0.023 (2)	0.017 (2)	0.022 (2)	0.0001 (19)	0.0000 (19)	−0.0059 (18)
C6	0.025 (2)	0.023 (2)	0.025 (2)	−0.002 (2)	−0.003 (2)	−0.0097 (19)
C5	0.022 (2)	0.018 (2)	0.029 (2)	−0.0011 (19)	−0.008 (2)	−0.0029 (19)
C2	0.023 (2)	0.016 (2)	0.022 (2)	0.0010 (19)	−0.0046 (18)	−0.0052 (18)

Cl1	0.0244 (6)	0.0273 (6)	0.0235 (5)	0.0001 (5)	−0.0081 (4)	−0.0108 (4)

Geometric parameters (Å, º)

N2—C6	1.225 (7)	C3—C4	1.437 (7)
N1—C5	1.371 (7)	C3—C6	1.473 (8)
N1—C1	1.379 (6)	C4—C5	1.398 (8)
N1—H1	0.8999	C4—H4A	0.9500
C1—C2	1.404 (8)	C5—H5A	0.9500
C1—H1A	0.9500	C2—H2A	0.9500
C3—C2	1.430 (7)		
C5—N1—C1	122.5 (5)	C5—C4—H4A	121.0
C5—N1—H1	118.8	C3—C4—H4A	121.0
C1—N1—H1	118.8	N2—C6—C3	177.9 (5)
N1—C1—C2	119.9 (5)	N1—C5—C4	120.7 (4)
N1—C1—H1A	120.0	N1—C5—H5A	119.6
C2—C1—H1A	120.0	C4—C5—H5A	119.6
C2—C3—C4	120.3 (5)	C1—C2—C3	118.5 (4)
C2—C3—C6	118.9 (4)	C1—C2—H2A	120.7
C4—C3—C6	120.8 (5)	C3—C2—H2A	120.7
C5—C4—C3	118.1 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1^{i}	0.90	2.14	3.033 (5)	174
C4—H4*A*···Cl1	0.95	2.71	3.566 (5)	151
C5—H5*A*···Cl1^{ii}	0.95	2.65	3.566 (6)	161

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