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4-Acetylpyridinium chloride

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Key indicators

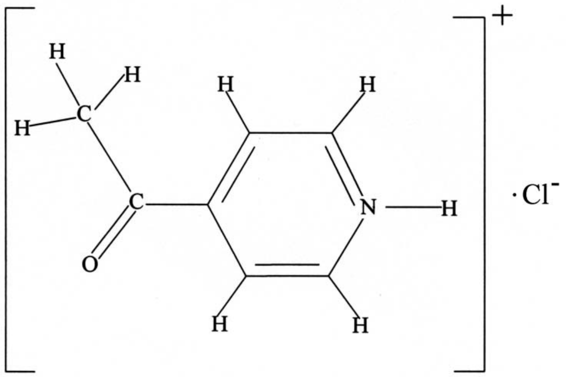
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.073
wR factor = 0.179
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of 4-acetylpyridinium chloride, $C_7H_8NO^+\cdot Cl^-$, consists of organic layers and Cl^- anions, which lie within these layers. A hydrogen-bonding network of N—H···Cl interactions stabilizes the structure.

Comment

The title compound is a salt containing a protonated 4-acetylpyridine cation and a Cl^- anion (Fig. 1). The projection of the crystal packing along the *b* axis is shown in Fig. 2. In the acetyl group, the O—C7 bond length is 1.214 (4) Å and the C7—C8 bond length is 1.482 (5) Å. Other bond lengths of the pyridine moiety are consistent with the literature data. 4-Acetylpyridine can form complexes with metals, for example with Zn (Steffen & Palenik, 1977) or Ni (Pang *et al.*, 1994). The structure of 4-acetylpyridine with pentachlorophenol is also known (Majerz *et al.*, 1991). The Cl^- anions and the 4-acetylpyridinium ions in the title compound are bonded by medium-strong hydrogen bonds, which stabilize the molecules in the crystal structure.



(I)

Experimental

4-Acetylpyridine was obtained according to the method described by Piner (1934). All reagents and solvents were used as purchased without further purification. 4-Acetylpyridinium chloride was prepared by the dropwise addition of concentrated HCl (36%, Aldrich; 50 ml) to an aqueous solution (10 ml) of 4-acetylpyridine (1 g). The solution was heated to 333 K and stirred for about 2 h. After cooling, the precipitate was filtered off. Good quality single crystals were obtained by recrystallization from an aqueous methanol solution (1:1) at room temperature. IR (KBr, ν, cm^{-1}): 3228, 2950, 2280, 1960, 1476, 1295, 1170, 843, 600, 585. Analysis calculated for C_7H_8ClNO: C 53.35, H 4.79, N 8.88, Cl 22.49%, found: C 52.78, H 3.23, N 8.15, Cl 22.12%.

doi:10.1107/S1600536805006872

Crystal data

$C_7H_8NO^+\cdot Cl^-$
$M_r = 157.59$
Monoclinic, $P2_1/c$
$a = 8.442\ (2)$ Å
$b = 7.117\ (1)$ Å
$c = 13.162\ (3)$ Å
$\beta = 103.76\ (3)^\circ$
$V = 768.1\ (3)$ Å^3
$Z = 4$
$D_x = 1.363$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 935 reflections
$\theta = 3.2$–27.5°
$\mu = 0.43$ mm^{-1}
$T = 298\ (2)$ K
Lath, yellow
$0.34 \times 0.12 \times 0.08$ mm

Data collection

Kuma KM-4 CCD diffractometer
ω scans
Absorption correction: numerical (*CrysAlis RED*; Oxford Diffraction, 2004)
$T_{\min} = 0.783$, $T_{\max} = 0.930$
5016 measured reflections
1731 independent reflections
1042 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.145$
$\theta_{\max} = 27.5^\circ$
$h = -10 \rightarrow 10$
$k = -7 \rightarrow 9$
$l = -17 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.179$
$S = 1.10$
1731 reflections
96 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N—H1$\cdots$Cl	1.04 (5)	1.98 (5)	2.997 (3)	164 (4)
C6—H6$\cdots$Cl$^{\rm i}$	0.93	2.68	3.544 (4)	154
C6—H6$\cdots$O$^{\rm ii}$	0.93	2.48	2.907 (4)	108

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

The H atom bonded to the N atom was placed at the position observed in a Fourier map and refined isotropically. Other H atoms were placed in calculated positions, with C—H distances of 0.93 or 0.96 Å, and were refined using a riding model with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C).

Data collection: *KM-4 CCD* (Oxford Diffraction, 2004); cell refinement: *KM-4 CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

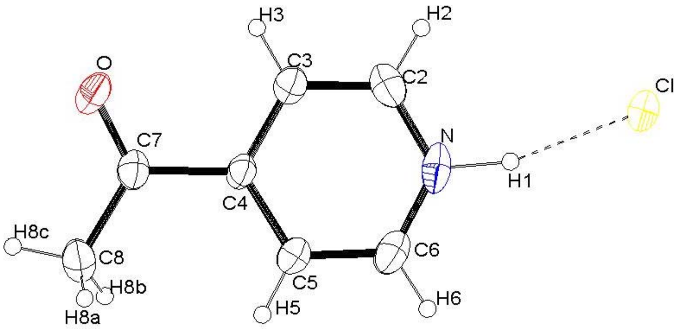


Figure 1
View of the asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond

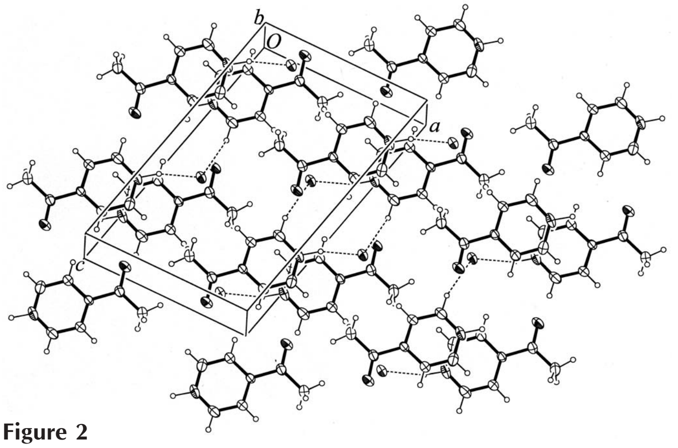


Figure 2
Crystal packing viewed approximately along the *b* axis. Dashed lines indicate hydrogen bonds.

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