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4-Amino-(1-carboxymethyl)pyridinium chloride

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Key indicators

Single-crystal X-ray study
T = 115 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.107
Data-to-parameter ratio = 18.1

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

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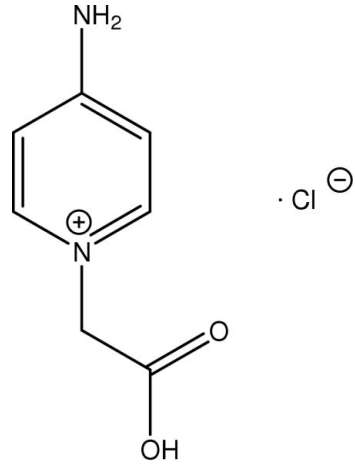
In the title structure, $C_7H_9N_2O_2^+\cdot Cl^-$, the dihedral angle between the pyridinium ring and carboxymethylene group is 70.5 (1)°. The anions and cations are interconnected by intermolecular N—H···Cl and O—H···Cl hydrogen bonds, forming a three-dimensional network.

Comment

It is known that pyridinium derivatives have antibacterial and antifungal activities (Sliwa & Mianowska, 1989). In a continuation of our studies of pyridinium derivatives, the crystal structure analysis of (I), has been undertaken.



(I)

The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles in (I) are comparable with those in related structures (Seethalakshmi *et al.*, 2006*a*,*b*). In (I), the dihedral angle between the planes of pyridinium ring and carboxymethylene unit is 70.5 (1)°. In the crystal structure, atom N2 acts as a donor for an intermolecular N—H···Cl hydrogen bond with two different symmetry-related chloride anions (Table 1), while hydroxy atom O1 is involved in an intermolecular O—H···Cl hydrogen bond. The combination of the N—H···Cl and O—H···Cl hydrogen bonds connects anions and cations into a three-dimensional network (Fig. 2).

Experimental

A solution of 4-aminopyridine (1.17 g, 25 ml) and 1-chloroacetic acid (1.188 g, 25 ml) in dry acetone was stirred for 2 h at room temperature (303 K). The resulting solid was filtered off and washed with dry acetone to give (I), which was recrystallized from an aqueous ethanol (80% *v*/*v*) solution.

Crystal data

$C_7H_9N_2O_2^+\cdot Cl^-$
M_r = 188.61
Orthorhombic, $P2_12_12_1$
a = 4.4324 (5) Å
b = 8.8524 (10) Å
c = 21.431 (3) Å
V = 840.90 (18) Å^3
Z = 4
D_x = 1.490 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 115 (2) K
Needle fragment, colourless
0.25 × 0.12 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer with an Cryosystems Oxford Cryostream cooler
ω scans with κ offsets
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.904, T_{max} = 0.960
18548 measured reflections
2149 independent reflections
1900 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 28.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
S = 1.11
2149 reflections
119 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.092P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}
Absolute structure: Flack (1983), 859 Friedel pairs
Flack parameter: 0.32 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···Cl1	0.74 (3)	2.24 (3)	2.9712 (16)	169 (3)
N2—H1*N*···Cl1^{i}	0.83 (3)	2.41 (3)	3.226 (2)	168 (3)
N2—H2*N*···Cl1^{ii}	0.92 (3)	2.34 (3)	3.252 (2)	174 (2)

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (ii) $-x+\frac{1}{2}, -y+1, z-\frac{1}{2}$.

The amino and hydroxy H atoms were located in a difference Fourier map and refined with U_{iso}(H) = 1.2U_{eq}(N) and 1.5U_{eq}(O), respectively. The remaining H atoms were placed in geometrically idealized positions (C—H = 0.95–0.99 Å) and were constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C). The crystal is an inversion twin with unequal components.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Version 1.07; Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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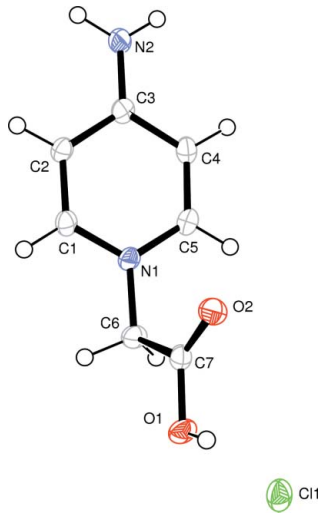

Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

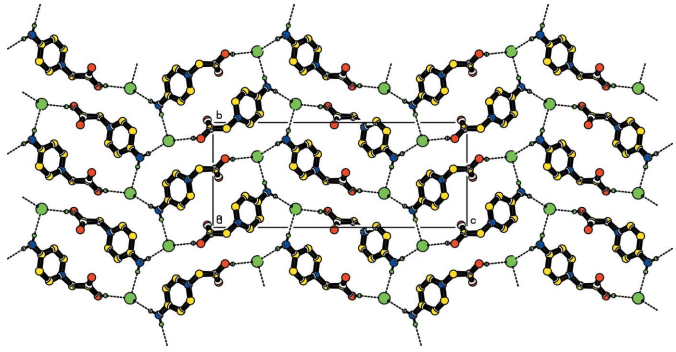

Figure 2
Part of the crystal structure of (I), viewed along the *a* axis. Intermolecular N—H···Cl and O—H···Cl hydrogen bonds are indicated by dashed lines. All the H atoms, except those involved in hydrogen bonding, have been omitted for clarity.

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