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## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.046  
 $wR$  factor = 0.123  
Data-to-parameter ratio = 15.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Isonipecotate chloride

The structure of the title compound,  $\text{C}_6\text{H}_{12}\text{NO}_2^+\cdot\text{Cl}^-$ , consists of an isonipecotate cation and a  $\text{Cl}^-$  anion linked by intermolecular  $\text{O}-\text{H}\cdots\text{Cl}$  and  $\text{N}-\text{H}\cdots\text{Cl}$  interactions into a three-dimensional network structure.Received 3 January 2006  
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## Comment

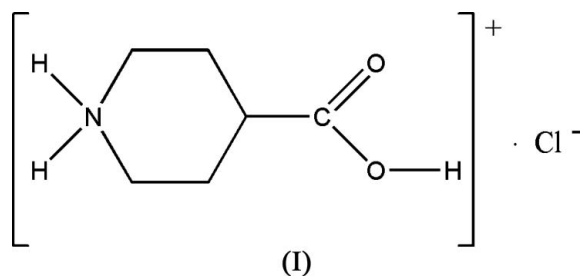
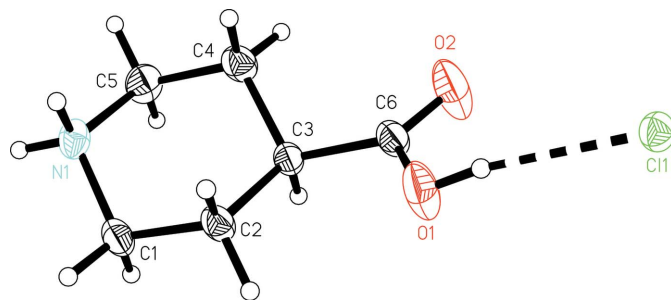
In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Directional intermolecular interactions are the primary tools in achieving this goal (Zaworotko, 1997; Braga & Grepioni, 2000).The title compound, (I), consists of a isonipecotate cation and a  $\text{Cl}^-$  anion (Fig. 1). The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The ring (N1/C1–C5) is not planar, having a total puckering amplitude  $Q_T = 0.571(2)\text{ \AA}$  (Cremer & Pople, 1975) and a distorted chair form [ $\varphi = 157.9(3)^\circ$  and  $\theta = 177.9(3)^\circ$ ]. It has a pseudo-mirror plane passing through atoms N1 and C3, as can be deduced from the torsion angles (Table 1).In the crystal structure of (I), there are multiple intermolecular interactions, such as  $\text{O}-\text{H}\cdots\text{Cl}$  and  $\text{N}-\text{H}\cdots\text{Cl}$  (Table 2, Fig. 2), generating a three-dimensional network structure (Fig. 2).

Figure 1

The structure of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The  $\text{O}-\text{H}\cdots\text{Cl}$  interaction is shown by a dashed line.

## Experimental

The title compound was synthesized by the hydrothermal method from a mixture of isonipecotic acid (0.04 g, 0.3 mmol), 2,2'-bipyridine (0.05 g, 0.3 mmol), copper(II) chloride dihydrate (0.05 g, 0.3 mmol) and water (8.0 ml) in a Teflon-lined stainless steel reactor (15.0 ml). The solution was heated at 423 K for 4 d. After reaction, the vessel was slowly cooled to room temperature to give colourless crystals of (I) (yield 0.012 g, 30%; m.p. 521–522 K).

## Crystal data

$C_6H_{12}NO_2^+ \cdot Cl^-$   
 $M_r = 165.62$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 7.0405$  (7) Å  
 $b = 7.4902$  (7) Å  
 $c = 15.2806$  (15) Å  
 $V = 805.82$  (14) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.365$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 352 reflections  
 $\theta = 2.7$ – $25.1^\circ$   
 $\mu = 0.42$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Block, colourless  
 $0.36 \times 0.31 \times 0.18$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: numerical (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.86$ ,  $T_{\max} = 0.93$   
 3980 measured reflections

1426 independent reflections  
 1394 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.016$   
 $\theta_{\text{max}} = 25.1^\circ$   
 $h = -6 \rightarrow 8$   
 $k = -8 \rightarrow 8$   
 $l = -18 \rightarrow 18$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.123$   
 $S = 1.20$   
 1426 reflections  
 92 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.4526P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.76$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), with 568 Friedel pairs  
 Flack parameter: 0.40 (13)

Table 1

Selected geometric parameters (Å, °).

O1—C6	1.293 (4)	C3—C6	1.511 (4)
N1—C5	1.486 (5)	O2—C6	1.202 (4)
C2—C1	1.511 (5)		
C5—N1—C1	111.8 (3)	C4—C3—C2	110.9 (3)
C1—C2—C3	110.9 (3)	O2—C6—O1	120.8 (3)
N1—C1—C2	110.6 (3)	O2—C6—C3	122.7 (3)
C6—C3—C4	110.5 (3)	O1—C6—C3	116.0 (3)
C6—C3—C2	113.8 (3)		
C5—N1—C1—C2	58.6 (4)	C1—N1—C5—C4	−58.7 (4)
C3—C2—C1—N1	−55.4 (4)	C2—C3—C4—C5	−54.8 (4)
C1—C2—C3—C4	53.9 (4)	N1—C5—C4—C3	56.8 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1B $\cdots$ Cl1 <sup>i</sup>	0.90	2.26	3.157 (3)	178
N1—H1A $\cdots$ Cl1 <sup>ii</sup>	0.90	2.34	3.184 (3)	156
O1—H1 $\cdots$ Cl1	0.82	2.20	3.016 (3)	172

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

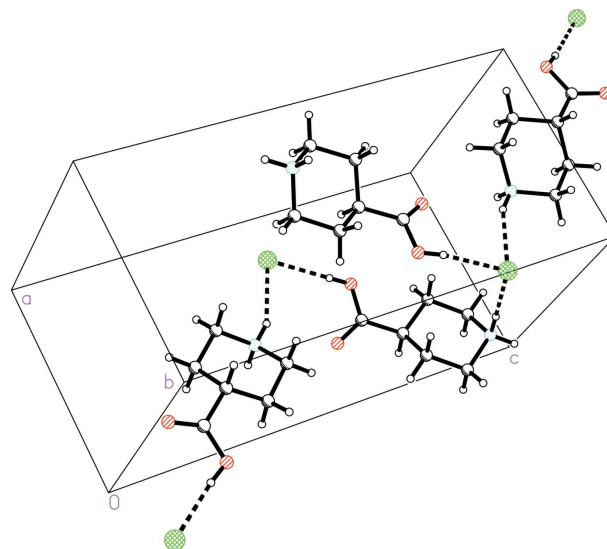


Figure 2

A packing diagram for (I). The O—H $\cdots$ Cl and N—H $\cdots$ Cl interactions are shown by dashed lines.

H atoms were positioned geometrically, with O—H = 0.82 Å, N—H = 0.90 Å, and C—H = 0.97 and 0.98 Å for methylene and methine H, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C,N,O})$ , where  $x = 1.5$  for hydroxyl H and  $x = 1.2$  for all other H. The value of the Flack parameter suggests inversion twinning.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPIII (Johnson & Burnett, 1996); software used to prepare material for publication: SHELXTL (Bruker, 2002).

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