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2-(Dihydroxymethyl)pyridinium chloride

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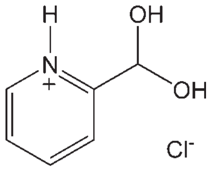
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.075; data-to-parameter ratio = 13.2.

In the title compound, $C_6H_8NO_2^+\cdot Cl^-$, intermolecular O—H···Cl and N—H···Cl hydrogen bonds are observed in which each chloride anion links three adjacent cations into a hydrogen-bond network.

Related literature

For a related compound, see Mantero *et al.* (2006).



Experimental

Crystal data

$C_6H_8NO_2^+\cdot Cl^-$
M_r = 161.58
Monoclinic, $P2_1/c$
a = 4.6879 (7) Å
b = 15.557 (2) Å
c = 10.1199 (14) Å
β = 91.181 (2)°
V = 737.88 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 291 K
0.12 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.948, T_{max} = 0.956
3676 measured reflections
1303 independent reflections
842 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.075
S = 0.89
1303 reflections
99 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···Cl1^{i}	0.85 (1)	2.24 (1)	3.089 (2)	176 (2)
O1—H1A···Cl1^{ii}	0.85 (1)	2.19 (1)	3.0374 (18)	177 (3)
N1—H1···Cl1^{iii}	0.86	2.33	3.115 (2)	151

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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: BG2326).

References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Mantero, D. G., Altaf, M., Neels, A. & Stoeckli-Evans, H. (2006). *Acta Cryst.* E**62**, o5204–o5206.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, o695   [**doi:10.1107/S1600536810006604**]

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H.-F. Qian and **W. Huang**

Comment

The crystal structure of pyridin-4-ylmethanediol, namely the hydrated form of isonicotinaldehyde has been previously reported (Mantero *et al.*, 2006). In this paper, we report the X-ray single-crystal structure of pyridin-2-ylmethanediol-1-ium chloride (I).

The molecular structure of (I) is illustrated in Fig. 1. The two hydroxyl groups lie at the same side of the aromatic ring. In the crystal packing, intermolecular O—H···Cl and N—H···Cl hydrogen bonding interactions are observed where every chloride anion links three adjacent molecules into a hydrogen-bond sustained network (Fig. 2).

Refinement

The H1A atom bonded with atom O1 was located in the difference synthesis and were refined isotropically. The other H atoms were placed in geometrically idealized positions and refined as riding, with C—H = 0.93–0.98 Å, N—H = 0.86 Å and O—H = 0.96 Å, U_{iso}(H) = 1.2U_{eq}(C), U_{iso}(H) = 1.2U_{eq}(N) and U_{iso}(H) = 1.5U_{eq}(O).

Figures

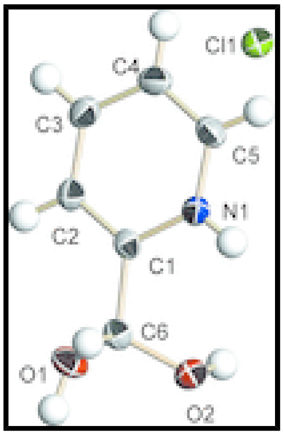

Fig. 1. The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

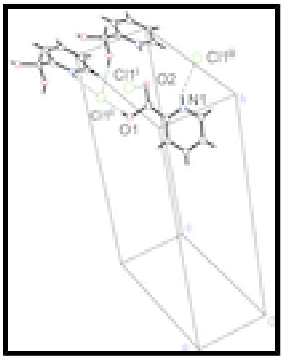

Fig. 2. Perspective view of the hydrogen bonding interactions in the crystal packing of (I), where the hydrogen bonds are shown as dashed lines. [Symmetry codes: (i) *x* - 1, -*y*+3/2, *z* + 1/2; (ii) *x*, *y*1/2, *z* + 1; (iii) *x*, -*y*+3/2, *z* + 1/2.]

2-(Dihydroxymethyl)pyridinium chloride

Crystal data

$C_6H_8NO_2^+\cdot Cl^-$

M_r = 161.58

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

a = 4.6879 (7) Å

b = 15.557 (2) Å

c = 10.1199 (14) Å

β = 91.181 (2)°

V = 737.88 (18) Å^3

Z = 4

$F(000)$ = 336

D_x = 1.455 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 776 reflections

θ = 2.4–21.0°

μ = 0.45 mm^{-1}

T = 291 K

Block, colourless

0.12 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

T_{min} = 0.948, T_{max} = 0.956

3676 measured reflections

1303 independent reflections

842 reflections with $I > 2\sigma(I)$

R_{int} = 0.058

θ_{max} = 25.0°, θ_{min} = 2.4°

$h = -5\rightarrow 5$

$k = -12\rightarrow 18$

$l = -12\rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.035

$wR(F^2)$ = 0.075

S = 0.89

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
1303 reflections	$(\Delta/\sigma)_{max} = 0.001$
99 parameters	$\Delta\rho_{max} = 0.22$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Experimental. The structure was solved by direct methods (Bruker, 2000) and successive difference Fourier syntheses.

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 $F^2 > \sigma(F^2)$ 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}
C1	0.0342 (4)	0.62701 (15)	0.8930 (2)	0.0395 (6)
C2	0.1167 (5)	0.54999 (16)	0.8429 (2)	0.0469 (6)
H2	0.2515	0.5168	0.8883	0.056*
C3	0.0002 (5)	0.52104 (16)	0.7246 (2)	0.0544 (7)
H3	0.0549	0.4681	0.6906	0.065*
C4	−0.1975 (5)	0.57099 (17)	0.6572 (2)	0.0553 (7)
H4	−0.2792	0.5519	0.5780	0.066*
C5	−0.2716 (5)	0.64860 (17)	0.7082 (2)	0.0504 (7)
H5	−0.4015	0.6836	0.6630	0.060*
C6	0.1322 (5)	0.66291 (15)	1.0257 (2)	0.0448 (6)
H6	0.0102	0.6382	1.0935	0.054*
Cl1	0.51126 (13)	0.65293 (4)	0.34503 (6)	0.0572 (2)
H1A	0.442 (6)	0.6405 (18)	1.1316 (11)	0.090 (11)*
H2A	0.211 (5)	0.7784 (16)	0.978 (2)	0.080 (11)*
N1	−0.1571 (4)	0.67433 (12)	0.82335 (17)	0.0424 (5)
H1	−0.2077	0.7233	0.8546	0.051*
O1	0.4092 (3)	0.63308 (12)	1.04924 (17)	0.0573 (5)
O2	0.1066 (4)	0.75152 (12)	1.03217 (17)	0.0567 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0371 (13)	0.0428 (15)	0.0389 (13)	−0.0011 (11)	0.0022 (11)	0.0061 (11)
C2	0.0486 (14)	0.0414 (15)	0.0508 (15)	0.0054 (12)	0.0005 (12)	0.0027 (12)
C3	0.0671 (17)	0.0424 (16)	0.0537 (17)	−0.0014 (14)	0.0030 (14)	−0.0052 (13)
C4	0.0661 (18)	0.0557 (18)	0.0439 (15)	−0.0126 (15)	−0.0050 (13)	−0.0025 (13)

C5	0.0529 (16)	0.0540 (17)	0.0441 (15)	−0.0023 (13)	−0.0062 (12)	0.0083 (13)
C6	0.0431 (14)	0.0467 (16)	0.0446 (14)	0.0032 (13)	0.0011 (11)	0.0031 (12)
Cl1	0.0683 (5)	0.0469 (4)	0.0559 (4)	−0.0043 (3)	−0.0107 (3)	−0.0036 (3)
N1	0.0464 (12)	0.0389 (12)	0.0418 (12)	0.0010 (10)	0.0008 (9)	0.0013 (9)
O1	0.0480 (11)	0.0753 (14)	0.0483 (12)	0.0133 (9)	−0.0086 (9)	−0.0063 (9)
O2	0.0670 (13)	0.0478 (12)	0.0551 (12)	0.0021 (10)	−0.0013 (10)	−0.0084 (9)

Geometric parameters (Å, °)

C1—N1	1.348 (3)	C5—N1	1.334 (3)
C1—C2	1.360 (3)	C5—H5	0.9300
C1—C6	1.518 (3)	C6—O2	1.385 (3)
C2—C3	1.381 (3)	C6—O1	1.395 (3)
C2—H2	0.9300	C6—H6	0.9800
C3—C4	1.379 (3)	N1—H1	0.8600
C3—H3	0.9300	O1—H1A	0.852 (10)
C4—C5	1.361 (3)	O2—H2A	0.853 (10)
C4—H4	0.9300		

N1—C1—C2	118.5 (2)	N1—C5—H5	120.1
N1—C1—C6	116.6 (2)	C4—C5—H5	120.1
C2—C1—C6	124.8 (2)	O2—C6—O1	113.84 (19)
C1—C2—C3	120.0 (2)	O2—C6—C1	112.52 (18)
C1—C2—H2	120.0	O1—C6—C1	106.99 (18)
C3—C2—H2	120.0	O2—C6—H6	107.7
C4—C3—C2	119.6 (2)	O1—C6—H6	107.7
C4—C3—H3	120.2	C1—C6—H6	107.7
C2—C3—H3	120.2	C5—N1—C1	123.0 (2)
C5—C4—C3	119.1 (2)	C5—N1—H1	118.5
C5—C4—H4	120.4	C1—N1—H1	118.5
C3—C4—H4	120.4	C6—O1—H1A	105.8 (19)
N1—C5—C4	119.7 (2)	C6—O2—H2A	114.0 (19)

N1—C1—C2—C3	−1.4 (3)	C2—C1—C6—O2	157.6 (2)
C6—C1—C2—C3	175.9 (2)	N1—C1—C6—O1	−150.91 (18)
C1—C2—C3—C4	0.6 (4)	C2—C1—C6—O1	31.8 (3)
C2—C3—C4—C5	0.8 (4)	C4—C5—N1—C1	0.7 (3)
C3—C4—C5—N1	−1.4 (4)	C2—C1—N1—C5	0.7 (3)
N1—C1—C6—O2	−25.2 (3)	C6—C1—N1—C5	−176.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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Fig. 1

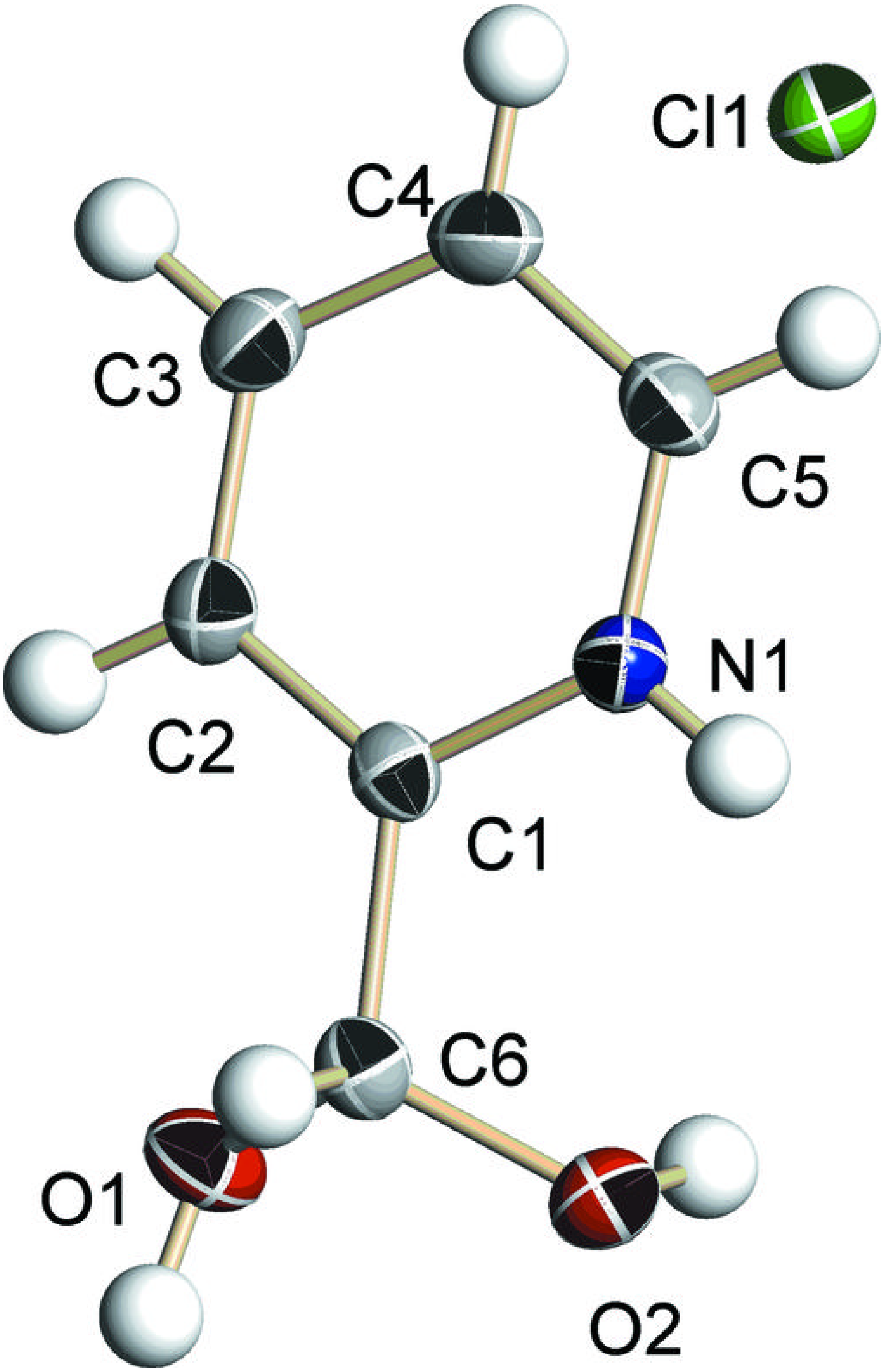

Fig. 2