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N-Hydroxy-*N*-methylammonium chloride

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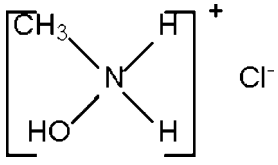
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(N–C) = 0.003 Å; R factor = 0.024; wR factor = 0.071; data-to-parameter ratio = 13.9.

In the crystal structure of the title compound, $CH_6NO^+\cdot Cl^-$, the cations and anions are linked by N–H···Cl and O–H···Cl hydrogen bonds into an undulating layer motif [Schläfli symbol: 4(8).6(8).8(2)]. All non-H atoms lie on a mirror plane.

Related literature

Only the cell dimensions of *N*-methyhydroxylammonium chloride have hitherto been reported; see: Toft & Jerslev (1967).



Experimental

Crystal data

$CH_6NO^+\cdot Cl^-$
M_r = 83.52
Orthorhombic, *Pbcm*
a = 7.8084 (3) Å
b = 8.7109 (3) Å
c = 6.0232 (1) Å
V = 409.69 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 100 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.839, T_{max} = 0.899
3330 measured reflections
558 independent reflections
493 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.070
S = 1.07
558 reflections
40 parameters
6 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O—H1···Cl	0.84 (1)	2.16 (1)	2.998 (1)	171 (2)
N—H2···Cl^{i}	0.88 (1)	2.33 (1)	3.1241 (4)	149 (1)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2008).

I thank the University of Malaya for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2270).

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supporting information

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S1. Comment

We are interested in the crystal structures of small organic molecules, molecules whose asymmetric unit consist of four or five non-hydrogen atoms only. *N*-Methylhydroxylammonium chloride (Scheme I) provides an example of such a system. However, the crystal structure is not known with only unit-cell dimensions reported (Toft & Jerslev, 1967).

The structure (Fig. 1) consists of cations and anions that are linked by N–H···Cl and O–H···Cl hydrogen bonds into an undulating layer motif [Schläfli symbol: 4(8).6(8).8(2)], Fig. 2 & Table 1. The non-hydrogen atoms lie on a mirror plane.

S2. Experimental

The chemical as purchased from the Aldrich Chemical Company was crystalline.

S3. Refinement

All hydrogen atoms were located in a difference Fouier map, and were refined with distance restraints (C–H 0.99±0.01, N–H 0.88±0.01 and O–H 0.84±0.01 Å). For the methyl group, an additional H···H = 1.59±0.01 Å was imposed. The temperature factors were freely refined.

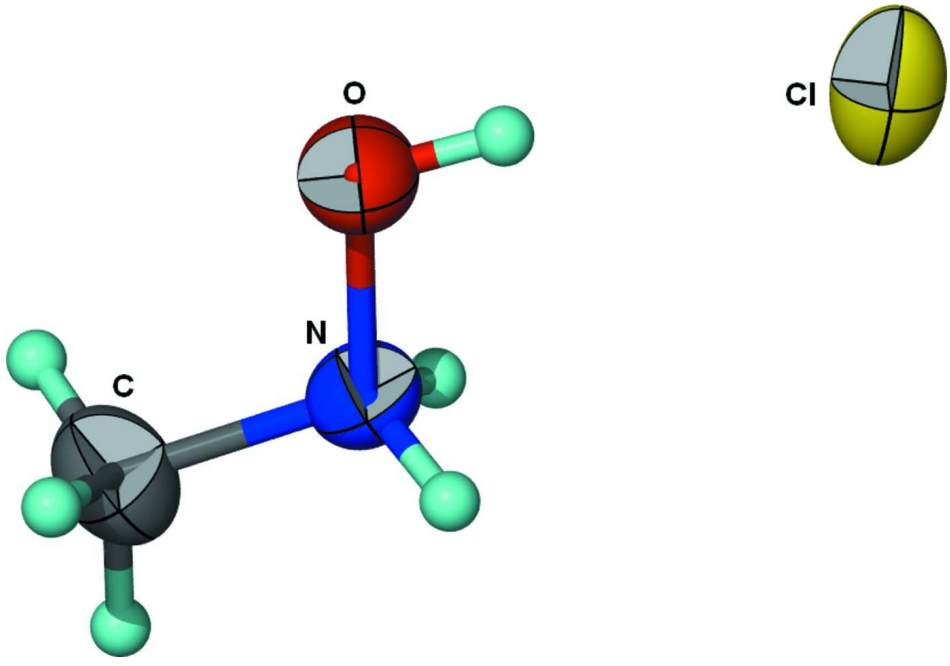

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of *N*-methylhydroxylammonium chloride at the 70% probability level.

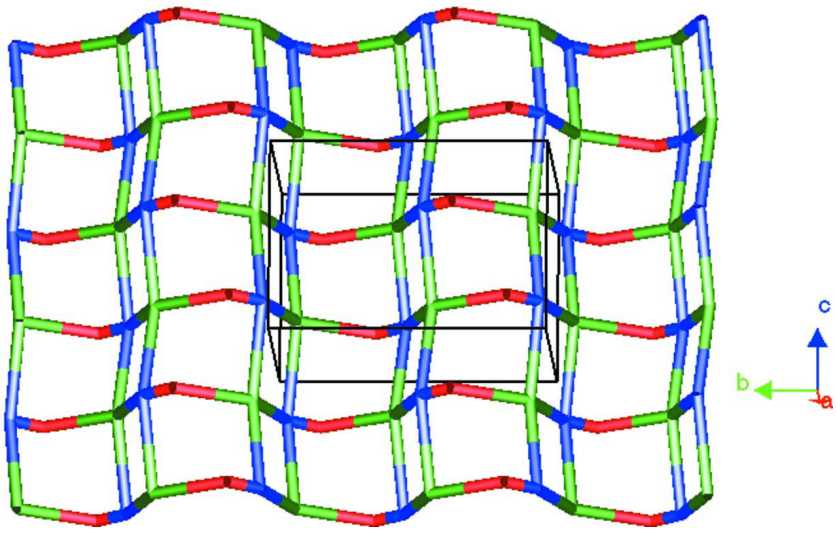

Figure 2

OLEX (Dolomanov *et al.*, 2003) representation of the hydrogen-bonded layer structure.

N-Hydroxy-*N*-methylammonium chloride

Crystal data

$CH_6NO^+ \cdot Cl^-$
$M_r = 83.52$
Orthorhombic, *Pbcm*
Hall symbol: -P 2c 2b
$a = 7.8084$ (3) Å
$b = 8.7109$ (3) Å
$c = 6.0232$ (1) Å
$V = 409.69$ (2) Å^3
$Z = 4$
$F(000) = 176$
$D_x = 1.354$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1402 reflections
$\theta = 2.6$–$28.2°$
$\mu = 0.73$ mm^{-1}
$T = 100$ K
Prism, colorless
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.839$, $T_{max} = 0.899$
3330 measured reflections
558 independent reflections
493 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.6°$
$h = -10 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.070$
$S = 1.07$
558 reflections
40 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.0529P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Extinction correction: *SHELXL*, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.15 (1)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl	0.35777 (6)	0.42790 (6)	0.2500	0.0433 (2)
O	0.1297 (2)	0.1511 (2)	0.2500	0.0389 (3)
N	0.2586 (2)	0.0376 (2)	0.2500	0.0300 (3)
C	0.1739 (3)	−0.1127 (3)	0.2500	0.0457 (5)
H1	0.184 (3)	0.2349 (17)	0.2500	0.048 (6)*
H2	0.3265 (17)	0.0482 (17)	0.366 (2)	0.041 (4)*
H3	0.2644 (18)	−0.190 (2)	0.2500	0.048 (6)*
H4	0.1075 (14)	−0.121 (2)	0.1170 (8)	0.064 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0455 (3)	0.0591 (4)	0.0254 (3)	−0.0196 (2)	0.000	0.000
O	0.0315 (7)	0.0324 (7)	0.0529 (8)	0.0032 (5)	0.000	0.000
N	0.0282 (6)	0.0336 (7)	0.0282 (7)	0.0016 (5)	0.000	0.000
C	0.053 (1)	0.033 (1)	0.051 (1)	−0.004 (1)	0.000	0.000

Geometric parameters (Å, º)

O—N	1.411 (2)	N—H2	0.88 (1)
N—C	1.467 (3)	C—H3	0.98 (1)
O—H1	0.84 (1)	C—H4	0.96 (1)
N—O—H1	104.5 (16)	N—C—H3	107.0 (12)
O—N—C	107.70 (14)	N—C—H4	108.0 (11)
O—N—H2	110.8 (10)	H3—C—H4	110.0 (9)
C—N—H2	111.3 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H1···Cl	0.84 (1)	2.16 (1)	2.998 (1)	171 (2)
N—H2···Cl^{i}	0.88 (1)	2.33 (1)	3.1241 (4)	149 (1)

Symmetry code: (i) *x*, −*y*+1/2, −*z*+1.