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N-Hydroxy-*N*-methylammonium chloride

Seik Weng Ng

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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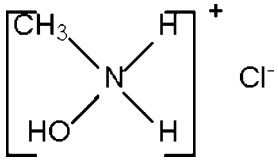
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(N–C) = 0.003 Å; R factor = 0.024; wR factor = 0.071; data-to-parameter ratio = 13.9.

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).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dolomanov, O. V., Blake, A. J., Champness, N. R. & Schröder, M. (2003). *J. Appl. Cryst.* **36**, 1283–1284.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Toft, L. & Jerslev, B. R. (1967). *Acta Chem. Scand.* **21**, 1383–1384.
Westrip, S. P. (2008). *publCIF*. In preparation.

supplementary materials

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N-Hydroxy-*N*-methylammonium chloride

S. W. Ng

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.

Experimental

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

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.

Figures

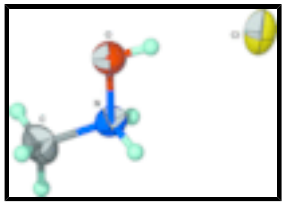

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of *N*-methylhydroxylammonium chloride at the 70% probability level.

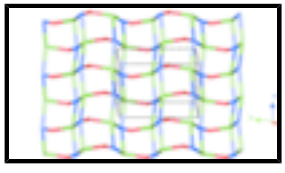

Fig. 2. *OLEX* (Dolomanov *et al.*, 2003) representation of the hydrogen-bonded layer structure.

N-Hydroxy-*N*-methylammonium chloride

Crystal data

$CH_6NO^+\cdot Cl^-$	$F_{000} = 176$
$M_r = 83.52$	$D_x = 1.354$ Mg m^{-3}

Orthorhombic, *Pbcm*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2c 2b	Cell parameters from 1402 reflections
a = 7.8084 (3) Å	θ = 2.6–28.2º
b = 8.7109 (3) Å	μ = 0.73 mm^{-1}
c = 6.0232 (1) Å	*T* = 100 (2) K
V = 409.69 (2) Å^3	Prism, colorless
Z = 4	0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer	558 independent reflections
Radiation source: fine-focus sealed tube	493 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 100(2) K	θ_{max} = 28.4º
ω scans	θ_{min} = 2.6º
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	*h* = −10→8
T_{min} = 0.839, T_{max} = 0.899	*k* = −11→11
3330 measured reflections	*l* = −8→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.024	All H-atom parameters refined
$wR(F^2)$ = 0.070	$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.0529P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
558 reflections	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
40 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
6 restraints	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.15 (1)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	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 (Å^2)

	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—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, °)

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 codes: (i) *x*, −*y*+1/2, −*z*+1.

Fig. 1

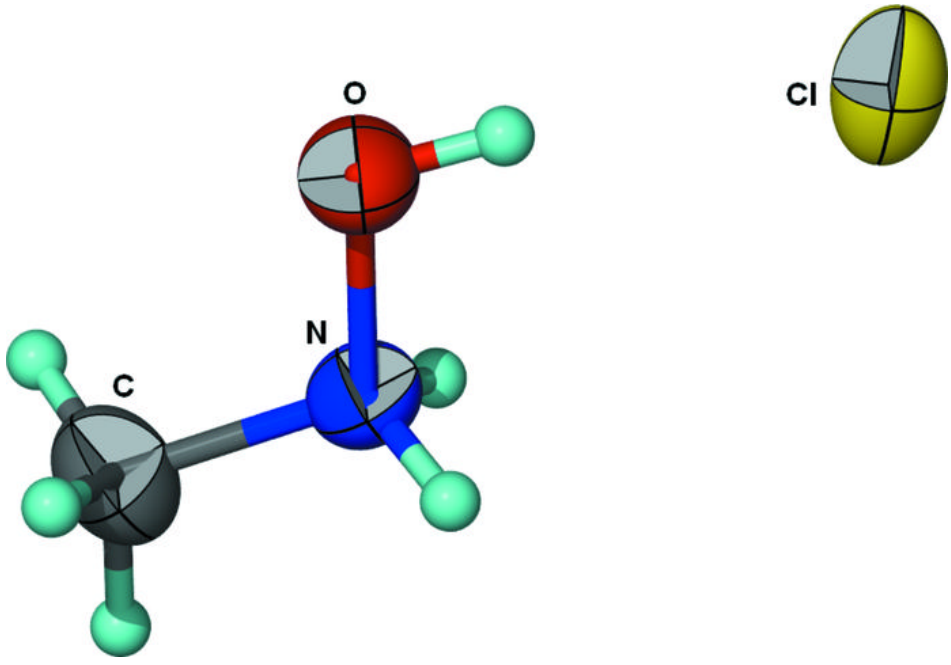

Fig. 2