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2-Methylanilinium chloride monohydrate

Meriem Benslimane,[a] Hocine Merazig,[a] Sofiane Bouacida,[b]* Sabrina Denbri,[a] Adel Beghidja[a] and Lahcène Ouahab[c]

[a]Laboratoire de Chimie Moléculaire, du Contrôle de l'Environnement et des Mesures Physico-chimiques, Faculté des Sciences Exactes, Département de Chimie, Université Mentouri, Constantine 25000, Algeria, [b]Département de Chimie, Faculté des Sciences et Sciences de l'Ingénieur, Université A. Mira de Béjaia, Route Targua Ouzmour 06000 Béjaia, Algeria, and [c]Organometallics and Molecular Materials, UMR 6226 CNRS Unité Sciences Chimiques de Rennes, Université de Rennes I, Avenue du Général Leclerc, 35042 Rennes, France
Correspondence e-mail: bouacida_sofiane@yahoo.fr

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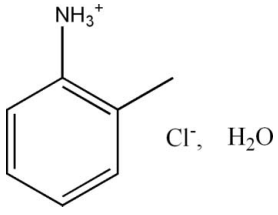
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.141; data-to-parameter ratio = 15.1.

The asymmetric unit of the title compound, $C_7H_{10}N^+\cdot Cl^-\cdot H_2O$, contains a 2-methylanilinium cation, a chloride anion and one molecule of water. The crystal structure consists of alternating layers of hydrophobic and hydrophilic zones of *o*-toluidine along the *c* axis. The water molecules and the chloride anions are sandwiched between these layers. A large number of cation–anion, cation–water and water–anion hydrogen bonds result in a two-dimensional network which reinforces the cohesion of the ionic structure.

Related literature

For related literature, see: Benali-Cherif *et al.* (2007); Bouacida *et al.* (2005*a*,*b*,*c*, 2006, 2007); Fábry *et al.* (2002); Hill (1998); Kagan *et al.* (1999); Koutselas *et al.* (1996); Mayer *et al.* (1999); Mazeaud *et al.* (2000); Mitzi *et al.* (1998); Muthamizhchelvan *et al.* (2005); Raptopoulou *et al.* (2002).



Experimental

Crystal data

$C_7H_{10}N^+\cdot Cl^-\cdot H_2O$
M_r = 161.63
Monoclinic, $P2_1/c$
a = 8.1871 (5) Å
b = 7.4046 (4) Å
c = 14.7415 (5) Å
β = 94.600 (4)°
V = 890.78 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 173 (2) K
0.10 × 0.08 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
2895 measured reflections
1508 independent reflections
1203 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.141
S = 1.11
1508 reflections
100 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1^{i}	0.89	2.29	3.1736 (18)	170
N1—H1B···Cl1^{ii}	0.89	2.39	3.2015 (17)	152
N1—H1C···O1W	0.89	1.82	2.704 (3)	175
O1W—H1W···Cl1	0.72 (3)	2.45 (2)	3.167 (2)	177.9 (14)
O1W—H2W···Cl1^{iii}	0.76 (3)	2.42 (3)	3.141 (2)	161 (3)

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2263).

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supplementary materials

Acta Cryst. (2007). E**63**, o3682-o3683 [**doi:10.1107/S1600536807037117**]

2-Methylanilinium chloride monohydrate

M. Benslimane, H. Merazig, S. Bouacida, S. Denbri, A. Beghidja and L. Ouahab

Comment

Organic–inorganic hybrid materials have attracted a great deal of attention over the past few decades (Koutselas *et al.*, 1996; Mitzi *et al.*, 1998; Mayer *et al.*, 1999; Mazeaud *et al.*, 2000) because of their ionic, electrical, magnetic and optical properties (Hill, 1998; Kagan *et al.*, 1999; Raptopoulou *et al.*, 2002).

The methylanilinium is already reported with nitrate (Benali-Cherif *et al.*, 2007), picrate (Muthamizhchelvan *et al.*, 2005) and dihydrogenphosphate (Fábry *et al.*, 2002).

In the course of our ongoing program related to the synthesis and structural study of hybrid compounds based on tin and amines (Bouacida *et al.*, 2007; Bouacida *et al.*, 2006; Bouacida *et al.*, 2005*a*; Bouacida *et al.*, 2005*b*; Bouacida *et al.*, 2005*c*), we report here the synthesis and crystal structure of 2-Methylanilinium chloride monohydrate, (I).

The molecular geometry and the atom-numbering scheme of (I) are shown in Fig. 1. The asymmetric unit of the title compound consist of a2-methylanilinium cation, a chloride anion and one molecule of water. The crystal structure consists of alternating layers of 2-methylanilinium. The chloride ions and water molecules are sandwiched between layers of hydrophobic and hydrophilic zones of 2-methylanilinium(Fig. 2). In this structure, three types of classical hydrogen bonds are observed, *viz*.cation–anion, cation–water and water-anion, with the N atom of the cation and O of water acting as donors (Fig.3, Table 1).

Experimental

Crystals were grown from aqueous solutions that were obtained by dissolving 1 mmol $SnCl_2{\cdot}2H_2O$, 2 mmol 2-methylaniline in hydrochloric acid. The solutions were slowly evaporated to dryness for a couple of weeks. Some red crystals were carefully isolated under polarizing microscope for analysis by X-ray diffraction.

Refinement

All H atoms were localized in Fourier maps but introduced in calculated positions and treated as riding on their parent C and N atoms with C—H = 0.93–0.96Å and N—H = 0.89Å and U_{iso}(H) =1.2–1.5 (carrier atom), except for H1W and H2W were located in a difference Fourier map and refined isotropically.

Figures

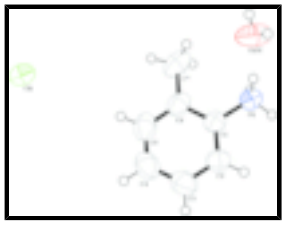

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

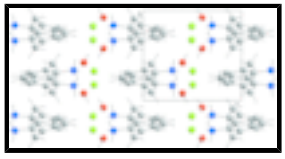

Fig. 2. The packing of (I), viewed down the C axis, showing layers of molecule.

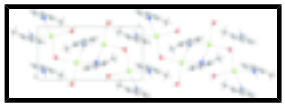

Fig. 3. A view of the ionic stacking, showing the hydrogen bonds as dashed lines.

2-Methylanilinium chloride monohydrate

Crystal data

$C_7H_{10}N^+\cdot Cl^-\cdot H_2O$	F_{000} = 344
M_r = 161.63	D_x = 1.205 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5072 reflections
a = 8.1871 (5) Å	θ = 1.0–25.0º
b = 7.4046 (4) Å	μ = 0.37 mm^{-1}
c = 14.7415 (5) Å	T = 173 (2) K
β = 94.600 (4)º	Prism, red
V = 890.78 (8) Å^3	0.10 × 0.08 × 0.06 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1203 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.016
T = 100(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: none	h = −9→9
2895 measured reflections	k = −8→8
1508 independent reflections	l = −16→16

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.141$

$S = 1.11$

1508 reflections

100 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0907P)^2 + 0.0493P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.27$ e Å^{-3}

$\Delta\rho_{min} = -0.19$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.116 (18)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2$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}
N1	0.2974 (2)	0.3362 (2)	0.44034 (12)	0.0545 (6)
C1	0.1203 (3)	0.3087 (3)	0.44239 (15)	0.0524 (7)
C2	0.0621 (3)	0.2488 (3)	0.52207 (15)	0.0606 (8)
C3	−0.1035 (3)	0.2160 (4)	0.5250 (2)	0.0759 (10)
C4	−0.2066 (3)	0.2427 (4)	0.4493 (2)	0.0818 (11)
C5	−0.1480 (4)	0.3034 (4)	0.3699 (2)	0.0791 (11)
C6	0.0189 (3)	0.3381 (3)	0.36395 (16)	0.0643 (9)
C7	0.0874 (4)	0.4069 (5)	0.27810 (17)	0.0932 (11)
O1W	0.4013 (3)	0.0788 (3)	0.32831 (14)	0.0917 (9)
Cl1	0.50523 (7)	0.17364 (8)	0.13149 (3)	0.0628 (3)
H1A	0.34565	0.32473	0.49634	0.0817*
H1B	0.31628	0.44633	0.41937	0.0817*
H1C	0.33783	0.25419	0.40409	0.0817*
H2	0.13360	0.23052	0.57350	0.0727*
H3	−0.14423	0.17583	0.57859	0.0910*
H4	−0.31794	0.21978	0.45120	0.0981*

H5	−0.22082	0.32174	0.31904	0.0949*
H7A	0.14965	0.51482	0.29157	0.1397*
H7B	−0.00103	0.43297	0.23328	0.1397*
H7C	0.15715	0.31644	0.25498	0.1397*
H1W	0.424 (3)	0.098 (3)	0.2830 (17)	0.0500*
H2W	0.442 (3)	−0.008 (4)	0.3448 (16)	0.0500*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0624 (12)	0.0549 (11)	0.0463 (10)	0.0004 (8)	0.0053 (8)	−0.0004 (7)
C1	0.0586 (13)	0.0458 (12)	0.0527 (12)	0.0065 (9)	0.0035 (9)	−0.0069 (8)
C2	0.0653 (15)	0.0590 (14)	0.0581 (13)	0.0029 (11)	0.0096 (10)	−0.0041 (10)
C3	0.0702 (18)	0.0810 (18)	0.0789 (18)	−0.0004 (13)	0.0212 (13)	−0.0104 (13)
C4	0.0610 (16)	0.088 (2)	0.097 (2)	0.0064 (14)	0.0095 (14)	−0.0251 (16)
C5	0.0688 (17)	0.0814 (19)	0.0839 (19)	0.0181 (13)	−0.0132 (14)	−0.0224 (13)
C6	0.0764 (17)	0.0592 (14)	0.0559 (14)	0.0133 (11)	−0.0042 (11)	−0.0084 (9)
C7	0.117 (2)	0.104 (2)	0.0556 (16)	0.0058 (19)	−0.0109 (14)	0.0130 (14)
O1W	0.142 (2)	0.0740 (13)	0.0642 (12)	0.0295 (13)	0.0406 (12)	0.0094 (10)
Cl1	0.0757 (5)	0.0641 (5)	0.0492 (4)	0.0006 (3)	0.0085 (3)	−0.0042 (2)

Geometric parameters (Å, °)

O1W—H1W	0.72 (3)	C4—C5	1.376 (4)
O1W—H2W	0.76 (3)	C5—C6	1.400 (4)
N1—C1	1.467 (3)	C6—C7	1.513 (4)
N1—H1B	0.8900	C2—H2	0.9300
N1—H1A	0.8900	C3—H3	0.9300
N1—H1C	0.8900	C4—H4	0.9300
C1—C2	1.376 (3)	C5—H5	0.9300
C1—C6	1.386 (3)	C7—H7C	0.9600
C2—C3	1.381 (3)	C7—H7A	0.9600
C3—C4	1.359 (4)	C7—H7B	0.9600
Cl1···N1^{i}	3.2015 (17)	C6···C2^{v}	3.578 (3)
Cl1···O1W	3.167 (2)	C7···H1C	2.8800
Cl1···N1^{ii}	3.1736 (18)	C7···H1B	2.7000
Cl1···O1W^{iii}	3.141 (2)	H1A···Cl1^{iv}	2.2900
Cl1···H2W^{iii}	2.42 (3)	H1A···H2	2.2600
Cl1···H1W	2.45 (2)	H1B···C7	2.7000
Cl1···H1A^{ii}	2.2900	H1B···Cl1^{iii}	2.3900
Cl1···H1B^{i}	2.3900	H1B···H7A	2.2900
O1W···C1	3.412 (3)	H1C···H7C	2.5900
O1W···Cl1	3.167 (2)	H1C···H2W	2.3200
O1W···N1	2.704 (3)	H1C···C7	2.8800
O1W···Cl1^{i}	3.141 (2)	H1C···H1W	2.2900
O1W···H7C	2.8100	H1C···O1W	1.8200
O1W···H1C	1.8200	H1W···H1C	2.2900

N1···O1W	2.704 (3)	H1W···Cl1	2.45 (2)
N1···Cl1^{iv}	3.1736 (18)	H2···H1A	2.2600
N1···Cl1^{iii}	3.2015 (17)	H2W···Cl1^{i}	2.42 (3)
N1···H7C	2.8800	H2W···H1C	2.3200
N1···H7A	2.7600	H5···H7B	2.4200
C1···O1W	3.412 (3)	H7A···H1B	2.2900
C1···C3^{v}	3.556 (4)	H7A···N1	2.7600
C2···C6^{v}	3.578 (3)	H7B···H5	2.4200
C2···C3^{vi}	3.533 (4)	H7C···O1W	2.8100
C3···C2^{vi}	3.533 (4)	H7C···N1	2.8800
C3···C1^{v}	3.556 (4)	H7C···H1C	2.5900
H1W—O1W—H2W	109 (3)	C5—C6—C7	122.9 (2)
H1B—N1—H1C	109.00	C3—C2—H2	120.00
C1—N1—H1C	109.00	C1—C2—H2	120.00
C1—N1—H1A	109.00	C2—C3—H3	120.00
C1—N1—H1B	110.00	C4—C3—H3	120.00
H1A—N1—H1B	109.00	C5—C4—H4	120.00
H1A—N1—H1C	109.00	C3—C4—H4	120.00
C2—C1—C6	122.5 (2)	C4—C5—H5	119.00
N1—C1—C6	119.2 (2)	C6—C5—H5	119.00
N1—C1—C2	118.2 (2)	C6—C7—H7B	109.00
C1—C2—C3	119.4 (2)	C6—C7—H7C	109.00
C2—C3—C4	119.7 (3)	C6—C7—H7A	109.00
C3—C4—C5	120.7 (3)	H7A—C7—H7C	109.00
C4—C5—C6	121.5 (3)	H7B—C7—H7C	109.00
C1—C6—C5	116.2 (2)	H7A—C7—H7B	109.00
C1—C6—C7	120.9 (2)		
N1—C1—C2—C3	−177.9 (2)	C1—C2—C3—C4	0.2 (4)
C6—C1—C2—C3	0.1 (4)	C2—C3—C4—C5	−0.5 (4)
N1—C1—C6—C5	177.9 (2)	C3—C4—C5—C6	0.6 (5)
N1—C1—C6—C7	−3.1 (3)	C4—C5—C6—C1	−0.3 (4)
C2—C1—C6—C5	0.0 (3)	C4—C5—C6—C7	−179.3 (3)
C2—C1—C6—C7	179.0 (2)		

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) *x*, −*y*+1/2, *z*+1/2; (v) −*x*, −*y*+1, −*z*+1; (vi) −*x*, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···Cl1^{iv}	0.8900	2.2900	3.1736 (18)	170.00
N1—H1B···Cl1^{iii}	0.8900	2.3900	3.2015 (17)	152.00
N1—H1C···O1W	0.8900	1.8200	2.704 (3)	175.00
O1W—H1W···Cl1	0.72 (3)	2.45 (2)	3.167 (2)	177.9 (14)
O1W—H2W···Cl1^{i}	0.76 (3)	2.42 (3)	3.141 (2)	161 (3)

Symmetry codes: (iv) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (i) −*x*+1, *y*−1/2, −*z*+1/2.

Fig. 1

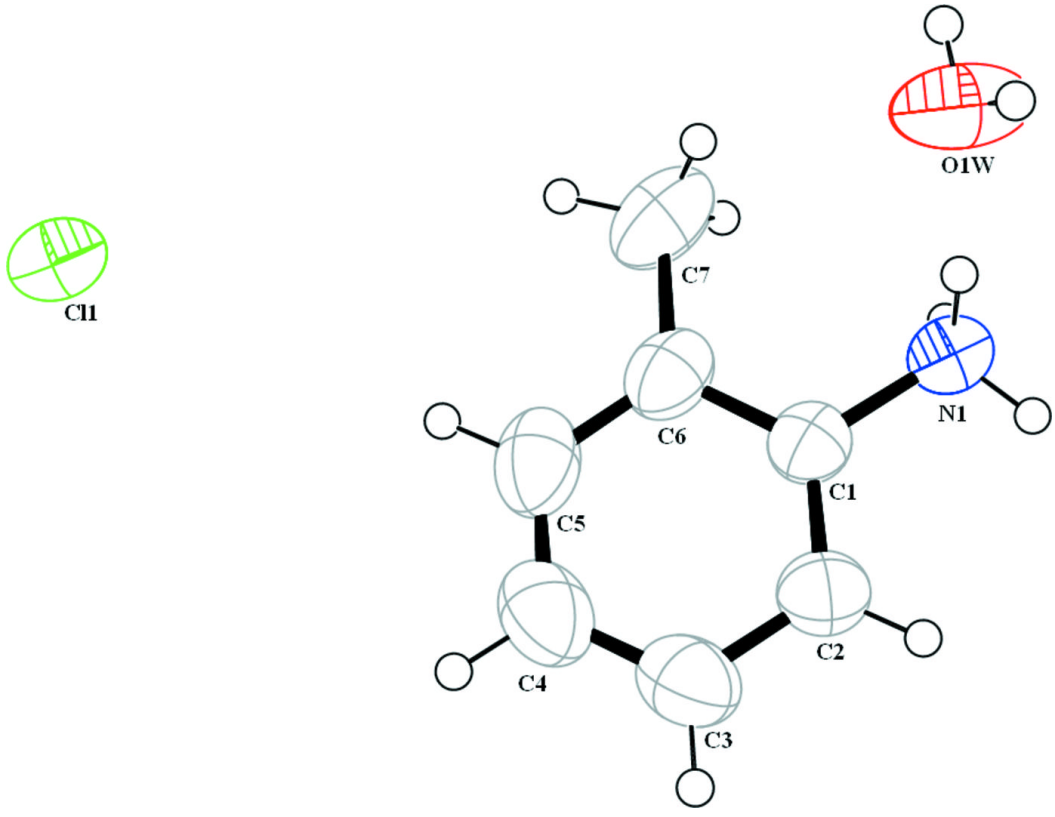

Fig. 2

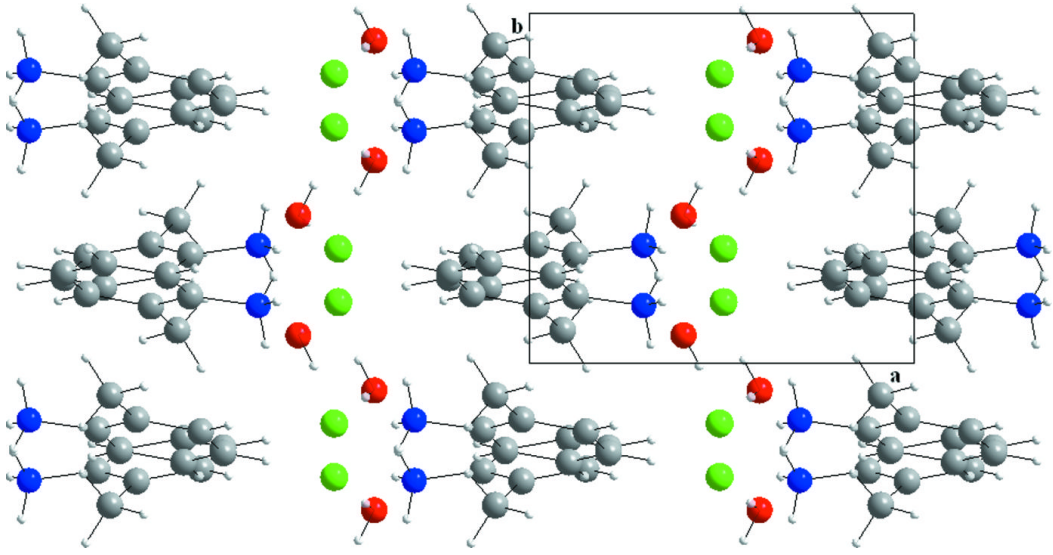

Fig. 3