

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 4-Methoxyanilinium chloride

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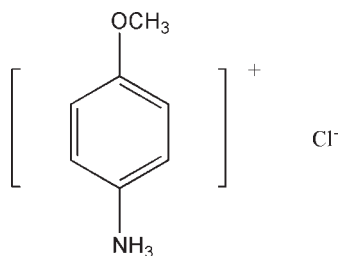
Received 5 August 2009; accepted 2 September 2009

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.062;  $wR$  factor = 0.165; data-to-parameter ratio = 20.7.

The crystal structure of the title compound,  $\text{C}_7\text{H}_{10}\text{NO}^+\cdot\text{Cl}^-$ , was synthesized by the reaction of 4-methoxyaniline and hydrochloric acid. In the crystal structure, the ions are involved in intermolecular  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds.

## Related literature

For a similar organic acid-base product, see: Wu *et al.* (2006). This work is part of a systematic investigation of dielectric-ferroelectric materials, including organic ligands, metal-organic coordination compounds and organic-inorganic hybrid materials; see: Li *et al.* (2008); Hang *et al.* (2009).



## Experimental

## Crystal data

$\text{C}_7\text{H}_{10}\text{NO}^+\cdot\text{Cl}^-$   
 $M_r = 159.61$

Orthorhombic,  $Pbca$   
 $a = 8.905$  (2) Å

$b = 8.489$  (2) Å  
 $c = 21.817$  (4) Å  
 $V = 1649.3$  (6) Å<sup>3</sup>  
 $Z = 8$

Mo  $K\alpha$  radiation  
 $\mu = 0.40$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.20 \times 0.20 \times 0.20$  mm

## Data collection

Rigaku SCXmini diffractometer  
Absorption correction: multi-scan  
(*CrystalClear*; Rigaku, 2005)  
 $T_{\min} = 0.924$ ,  $T_{\max} = 0.924$

15436 measured reflections  
1886 independent reflections  
1452 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.058$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.165$   
 $S = 1.12$   
1886 reflections

91 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.25$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.54$  e Å<sup>-3</sup>

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1D}\cdots\text{Cl1}^{\text{i}}$	0.89	2.47	3.360 (3)	179
$\text{N1}-\text{H1E}\cdots\text{Cl1}^{\text{ii}}$	0.89	2.50	3.209 (2)	137
$\text{N1}-\text{H1F}\cdots\text{Cl1}^{\text{iii}}$	0.89	2.38	3.167 (2)	147

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PRPKAPPA* (Ferguson, 1999).

The authors are grateful to the starter fund of Southeast University for financial support to buy the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2133).

## References

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## supporting information

*Acta Cryst.* (2009). E65, o2378 [doi:10.1107/S1600536809035429]

## 4-Methoxyanilinium chloride

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### S1. Comment

Acid-base reactions of organic reactands were already widely researched by ancient chemists (Wu *et al.*, 2006). This study is a part of a systematic investigation of dielectric-ferroelectric materials, including organic ligands, metal-organic coordination compounds and organic-inorganic hybrid materials (Li *et al.*, 2008; Hang *et al.*, 2009). Nevertheless, 4-methoxy-anilinium chloride shows no dielectric irregularity in the temperature range of 80 K to 400 K, (m.p. 401 K).

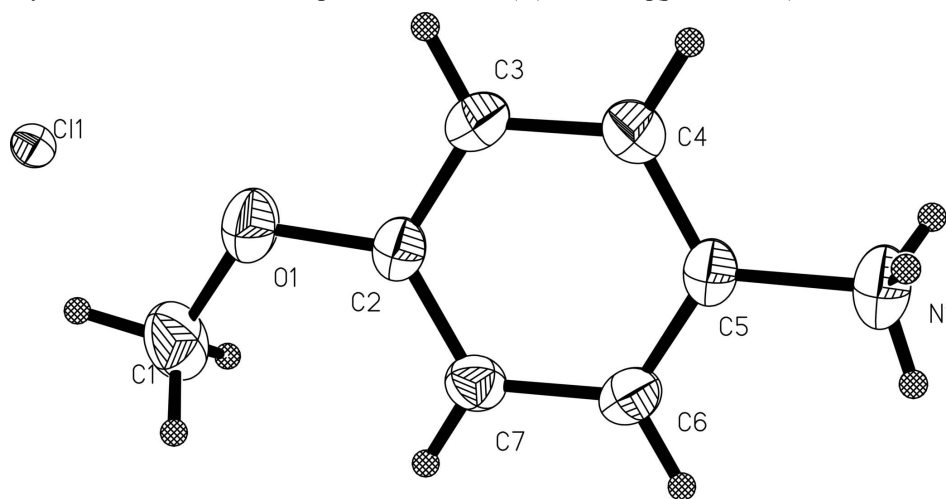
The asymmetric unit of the title compound is composed of cationic ( $\text{CH}_3\text{O}-\text{C}_6\text{H}_4-\text{NH}_3^+$ ) and chloride anions (Fig 1). Intramolecular hydrogen bonds between the ammonium groups of the organic cations and the chloride anions are observed in the crystal structure.

### S2. Experimental

Single crystals of 4-methoxy-anilinium chloride are prepared by slow evaporation at room temperature of 20 mL of an ethanolic solution of 4-methoxyphenylamine and an excess of hydrogen chloride (6 mol/L).

### S3. Refinement

All hydrogen atoms were calculated geometrically with C—H distances of 0.93 Å for aromatic C—H functions, 0.96 Å for the methyl group and 0.89 Å for the ammonium substituent. All hydrogen atoms were allowed to ride on the C and N atoms to which they are bonded with thermal parameters of  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$ .



**Figure 1**

The molecular structure of the title compound showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

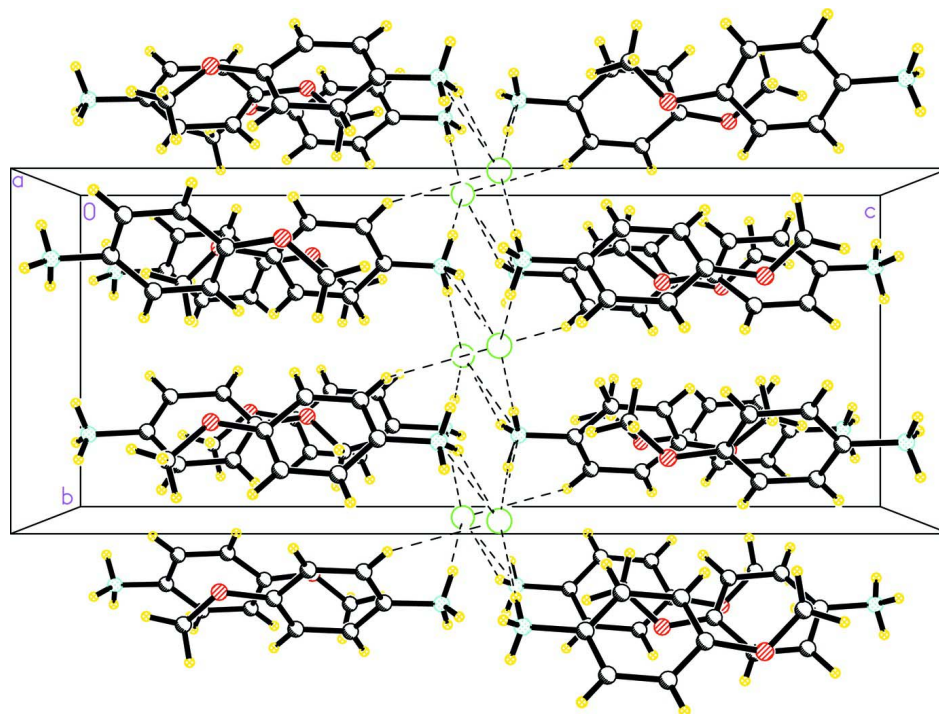


Figure 2

View of the packing of the title compound, stacking along the *a* axis. Dashed lines indicate hydrogen bonds.

#### 4-Methoxyanilinium chloride

##### Crystal data

$C_7H_{10}NO^+Cl^-$

$M_r = 159.61$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 8.905(2) \text{ \AA}$

$b = 8.489(2) \text{ \AA}$

$c = 21.817(4) \text{ \AA}$

$V = 1649.3(6) \text{ \AA}^3$

$Z = 8$

$F(000) = 672$

$D_x = 1.286 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 6458 reflections

$\theta = 3.0\text{--}27.6^\circ$

$\mu = 0.40 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Prism, colourless

$0.20 \times 0.20 \times 0.20 \text{ mm}$

##### Data collection

Rigaku SCXmini

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution:  $13.6612 \text{ pixels mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku, 2005)

$T_{\min} = 0.924$ ,  $T_{\max} = 0.924$

15436 measured reflections

1886 independent reflections

1452 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.058$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.4^\circ$

$h = -11 \rightarrow 11$

$k = -10 \rightarrow 11$

$l = -27 \rightarrow 28$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.165$   
 $S = 1.12$   
 1886 reflections  
 91 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0824P)^2 + 0.5018P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$

Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.75138 (6)	0.98509 (7)	0.52111 (3)	0.0470 (3)
O1	0.1534 (2)	0.1996 (2)	0.29469 (8)	0.0623 (6)
N1	0.0252 (3)	0.2494 (3)	0.04478 (10)	0.0617 (7)
H1D	-0.0468	0.3203	0.0383	0.093*
H1E	-0.0059	0.1553	0.0320	0.093*
H1F	0.1073	0.2770	0.0242	0.093*
C2	0.1175 (3)	0.2222 (3)	0.23454 (10)	0.0438 (6)
C5	0.0595 (3)	0.2423 (3)	0.11049 (11)	0.0441 (6)
C4	0.1677 (3)	0.1392 (3)	0.13138 (12)	0.0561 (7)
H4A	0.2203	0.0762	0.1039	0.067*
C6	-0.0179 (3)	0.3363 (3)	0.15081 (12)	0.0492 (6)
H6A	-0.0895	0.4069	0.1363	0.059*
C7	0.0108 (3)	0.3259 (3)	0.21326 (11)	0.0472 (6)
H7A	-0.0420	0.3890	0.2407	0.057*
C3	0.1970 (3)	0.1303 (4)	0.19295 (13)	0.0575 (7)
H3A	0.2710	0.0621	0.2071	0.069*
C1	0.0870 (4)	0.3025 (4)	0.33900 (13)	0.0761 (10)
H1A	0.1211	0.2740	0.3792	0.114*
H1B	-0.0203	0.2934	0.3371	0.114*
H1C	0.1157	0.4092	0.3304	0.114*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cl1	0.0461 (4)	0.0472 (4)	0.0478 (4)	-0.0017 (2)	0.0013 (3)	-0.0042 (2)

O1	0.0691 (13)	0.0735 (13)	0.0442 (10)	-0.0047 (11)	-0.0113 (9)	0.0042 (9)
N1	0.0690 (16)	0.0723 (16)	0.0439 (12)	-0.0200 (12)	-0.0091 (11)	0.0082 (11)
C2	0.0435 (14)	0.0466 (12)	0.0414 (13)	-0.0109 (11)	-0.0051 (10)	0.0065 (10)
C5	0.0440 (13)	0.0496 (13)	0.0388 (12)	-0.0143 (11)	-0.0040 (10)	0.0055 (10)
C4	0.0598 (16)	0.0597 (16)	0.0488 (15)	0.0083 (13)	0.0060 (12)	-0.0031 (12)
C6	0.0421 (13)	0.0499 (14)	0.0554 (14)	0.0024 (11)	-0.0056 (11)	0.0060 (12)
C7	0.0404 (13)	0.0526 (15)	0.0486 (13)	-0.0008 (11)	0.0000 (11)	-0.0056 (11)
C3	0.0570 (16)	0.0592 (16)	0.0564 (16)	0.0167 (14)	-0.0053 (13)	0.0062 (13)
C1	0.075 (2)	0.109 (3)	0.0448 (15)	-0.011 (2)	-0.0045 (14)	-0.0147 (16)

*Geometric parameters (Å, °)*

O1—C2	1.364 (3)	C4—C3	1.370 (4)
O1—C1	1.431 (4)	C4—H4A	0.9300
N1—C5	1.467 (3)	C6—C7	1.389 (4)
N1—H1D	0.8900	C6—H6A	0.9300
N1—H1E	0.8900	C7—H7A	0.9300
N1—H1F	0.8900	C3—H3A	0.9300
C2—C7	1.376 (4)	C1—H1A	0.9600
C2—C3	1.390 (4)	C1—H1B	0.9600
C5—C6	1.373 (4)	C1—H1C	0.9600
C5—C4	1.380 (4)		
C2—O1—C1	117.9 (2)	C5—C6—C7	119.9 (2)
C5—N1—H1D	109.5	C5—C6—H6A	120.0
C5—N1—H1E	109.5	C7—C6—H6A	120.0
H1D—N1—H1E	109.5	C2—C7—C6	119.9 (2)
C5—N1—H1F	109.5	C2—C7—H7A	120.0
H1D—N1—H1F	109.5	C6—C7—H7A	120.0
H1E—N1—H1F	109.5	C4—C3—C2	120.8 (2)
O1—C2—C7	125.2 (2)	C4—C3—H3A	119.6
O1—C2—C3	115.4 (2)	C2—C3—H3A	119.6
C7—C2—C3	119.4 (2)	O1—C1—H1A	109.5
C6—C5—C4	120.5 (2)	O1—C1—H1B	109.5
C6—C5—N1	119.8 (2)	H1A—C1—H1B	109.5
C4—C5—N1	119.6 (2)	O1—C1—H1C	109.5
C3—C4—C5	119.5 (2)	H1A—C1—H1C	109.5
C3—C4—H4A	120.3	H1B—C1—H1C	109.5
C5—C4—H4A	120.3		
C1—O1—C2—C7	-6.9 (4)	O1—C2—C7—C6	-178.8 (2)
C1—O1—C2—C3	173.4 (3)	C3—C2—C7—C6	0.9 (4)
C6—C5—C4—C3	0.4 (4)	C5—C6—C7—C2	0.4 (4)
N1—C5—C4—C3	-178.5 (2)	C5—C4—C3—C2	1.0 (4)
C4—C5—C6—C7	-1.1 (4)	O1—C2—C3—C4	178.1 (3)
N1—C5—C6—C7	177.8 (2)	C7—C2—C3—C4	-1.6 (4)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1D···C11 <sup>i</sup>	0.89	2.47	3.360 (3)	179
N1—H1E···C11 <sup>ii</sup>	0.89	2.50	3.209 (2)	137
N1—H1F···C11 <sup>iii</sup>	0.89	2.38	3.167 (2)	147

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