

## 4-Methoxy-3-nitropyridinium chloride

Daniel E. Lynch<sup>a\*</sup> and Ian McClenaghan<sup>b†</sup><sup>a</sup>School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England, and <sup>b</sup>Spa Contract Synthesis, School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England

† E-mail: 106355.1670@compuserve.com.

Correspondence e-mail: apx106@coventry.ac.uk

## Key indicators

Single-crystal X-ray study

T = 150 K

Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$ 

R factor = 0.043

wR factor = 0.121

Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The structure of the title compound,  $\text{C}_6\text{H}_7\text{N}_2\text{O}_3^+\cdot\text{Cl}^-$ , (I), comprises the hydrochloride salt of an essentially flat molecule with a single  $\text{N}-\text{H}\cdots\text{Cl}$  association. Two additional  $\text{C}-\text{H}\cdots\text{Cl}$  close contacts are also observed.

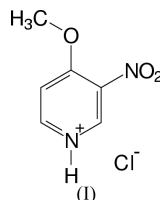
Received 18 December 2000

Accepted 19 December 2000

Online 22 December 2000

## Comment

The basified form of the title compound 4-methoxy-3-nitropyridinium chloride, (I), *i.e.* 4-methoxy-3-nitropyridine, is a useful intermediate in which the methoxy group can be readily replaced by nucleophiles. The molecule is also commercially available as the 4-ethoxy derivative but the methoxy version is less expensive. Both derivatives are prepared *via* the 4-chloro analogue, which is then treated with the appropriate alcohol. The 4-chloro compound has increased reactivity to nucleophiles but it is very lipophilic and corrosive to the skin, so it is much easier to handle as a 4-alkoxy compound.



## Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from a methanol solution.

## Crystal data

 $\text{C}_6\text{H}_7\text{N}_2\text{O}_3^+\cdot\text{Cl}^-$  $M_r = 190.59$ Monoclinic,  $P2_1/n$  $a = 10.6185 (4) \text{ \AA}$  $b = 7.1517 (4) \text{ \AA}$  $c = 11.3701 (5) \text{ \AA}$  $\beta = 111.523 (3)^\circ$  $V = 803.24 (6) \text{ \AA}^3$  $Z = 4$  $D_x = 1.576 \text{ Mg m}^{-3}$ Mo  $K\alpha$  radiation

Cell parameters from 4004

reflections

 $\theta = 2.9\text{--}27.5^\circ$  $\mu = 0.44 \text{ mm}^{-1}$  $T = 150 (2) \text{ K}$ 

Block, colourless

 $0.15 \times 0.15 \times 0.10 \text{ mm}$ 

## Data collection

Enraf-Nonius KappaCCD area-detector diffractometer

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SORTAV; Blessing, 1995)

 $T_{\min} = 0.937$ ,  $T_{\max} = 0.957$ 

5993 measured reflections

1835 independent reflections

1219 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.042$  $\theta_{\max} = 27.5^\circ$  $h = -13 \rightarrow 13$  $k = -8 \rightarrow 9$  $l = -13 \rightarrow 14$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.121$   
 $S = 1.00$   
 1835 reflections  
 114 parameters

H atoms treated by a mixture of  
 independent and constrained  
 refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0664P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

**Table 1**

 Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

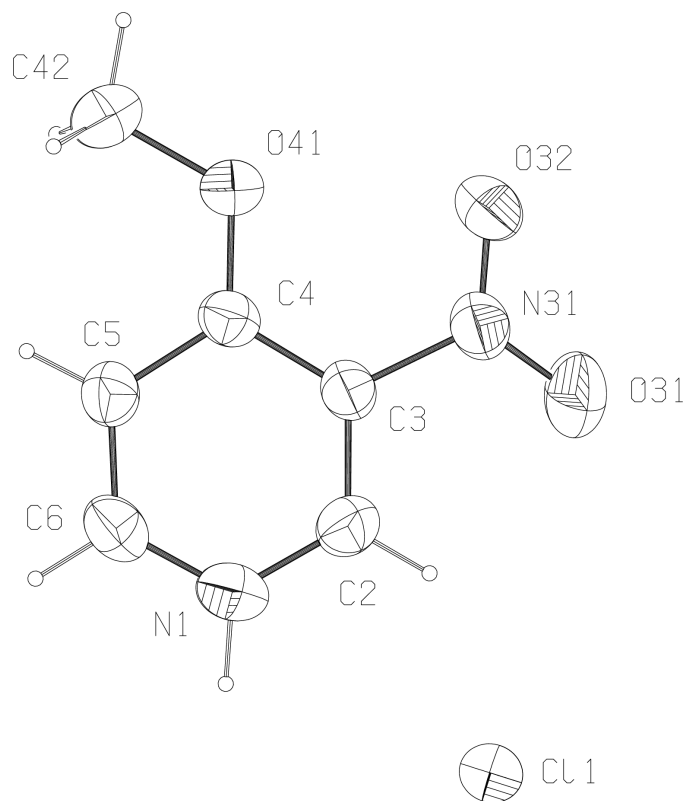
$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1 \cdots Cl1$	0.94 (3)	2.05 (3)	2.974 (2)	167 (2)
$C5-H5 \cdots Cl1^i$	0.95	2.74	3.629 (2)	157
$C6-H6 \cdots Cl1^{ii}$	0.95	2.58	3.521 (2)	173

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

All H atoms were included in the refinement at calculated positions as riding models, with C–H set to 0.95 (Ar–H) and 0.98  $\text{\AA}$  ( $\text{CH}_3$ ), except for the pyridinium H atom, which was located on difference syntheses and for which both positional and displacement parameters were refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the EPSRC National Crystallography Service (Southampton).



**Figure 1**  
 The molecular configuration and atom-numbering scheme for (I), showing 50% probability ellipsoids.

## References

- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–37.  
 Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.  
 Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307–326.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.