4-(Ethoxycarbonyl)anilinium chloride

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In the title crystal structure, $C_9H_{12}NO_2^+ \cdot Cl^-$, intermolecular $N-H \cdots Cl$ hydrogen bonds link cations and anions to form one-dimensional ladders propagating in the *a*-axis direction.

Comment

We are interested in biologically active esters and related ligands. Esters of 4-aminobenzoic acid can be used as local anaesthetics or as intermediate compounds in organic synthesis. Recent studies have revealed that some esters also show a broad range of biological activities (Fu & Liu, 1994). Furthermore, these types of esters can be used as coordinating ligands. As part of our ongoing studies (Jin & Xiao, 2005; Ma *et al.*, 2005), we report here the crystal structure of the title compound, (I).

(I)
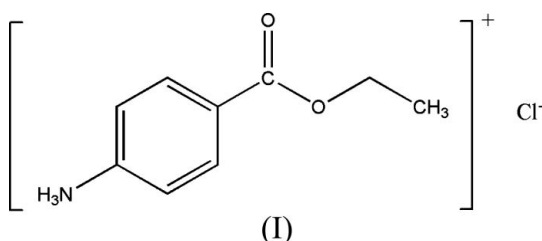
The asymmetric unit of (I) contains one ethyl 4-aminobenzoate cation and one chloride anion (Fig. 1). Bond lengths and angles in (I) show normal values (Allen *et al.*, 1987). The non-H atoms of the ethyl 4-aminobenzoate cation are essentially coplanar, with an r.m.s deviation of 0.025 Å.

In the crystal structure, intermolecular $N-H \cdots Cl$ hydrogen bonds link cations and anions to form one-dimensional ladders propagating in the *a* axis direction (Table 1 and Fig. 2).
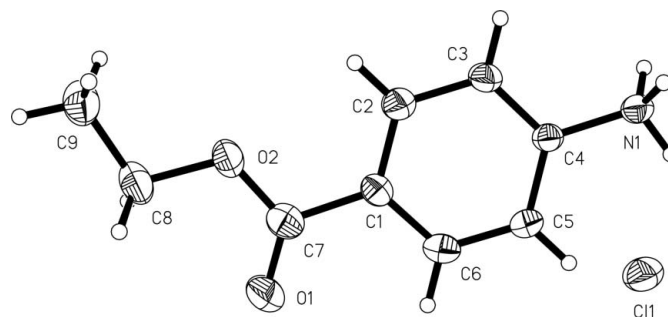
Figure 1
The asymmetric unit of (I), showing displacement ellipsoids at the 30% probability level.

Experimental

4-Aminobenzoic acid (1.00 g) and ethanol (40.0 ml) were added to a round-bottomed flask with a magnetic stirrer bar, and pure dry hydrogen chloride gas was passed into the mixture until it was saturated. The mixture was left overnight and then stirred for 4 h at 333 K (Dan, 2000), after which it was allowed to cool. The resulting white precipitate was filtered off and washed with ethanol and water. Colourless plate-like crystals of (I) were grown from an ethanol solution of the title compound by slow evaporation at room temperature.

Crystal data

$C_9H_{12}NO_2{}^+ \cdot Cl^-$
$M_r = 201.65$
Monoclinic, $P2_1/n$
$a = 6.0426 (18)$ Å
$b = 4.5978 (14)$ Å
$c = 37.005 (11)$ Å
$\beta = 91.820 (5)°$
$V = 1027.6 (5)$ Å^3

$Z = 4$
$D_x = 1.303$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.34$ mm^{-1}
$T = 292 (2)$ K
Needle, colourless
$0.60 \times 0.10 \times 0.02$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: ψ scan (SHELXTL; Bruker, 2001)
$T_{min} = 0.822$, $T_{max} = 0.993$

7676 measured reflections
1898 independent reflections
1200 reflections with $I > 2\sigma(I)$
$R_{int} = 0.100$
$\theta_{max} = 25.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.146$
$S = 0.98$
1898 reflections
128 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots Cl1^i$	0.895 (19)	2.34 (2)	3.200 (3)	162 (4)
$N1-H1B\cdots Cl1^{ii}$	0.882 (18)	2.40 (2)	3.216 (3)	154 (3)
$N1-H1C\cdots Cl1^{iii}$	0.906 (19)	2.21 (2)	3.111 (3)	171 (4)

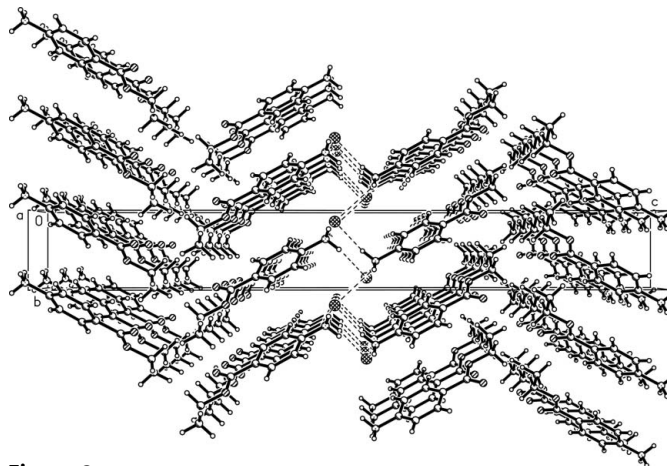Symmetry codes: (i) $x, y-1, z$; (ii) $x-1, y-1, z$; (iii) $-x+1, -y+1, -z$.

Figure 2
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

H atoms bonded to N atoms were located in a difference Fourier map and refined with $U_{iso}(H) = 1.5U_{eq}(N)$. All other H atoms were included in the riding-model approximation, with C—H distances of 0.93 (aromatic H atoms), 0.96 (methyl H atoms) and 0.97 Å (methylene H atoms), and with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for methyl H atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2001). *SMART* (Version 5.628), *SAINT* (Version 6.45) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
Dan, X.-X. (2000). *Practice Handbook of Synthsis of Fine Organic Chemicals*, pp. 130–131. Beijing: Chemical Industry Press.
Fu, X.-C. & Liu, Z.-Q. (1994). *Chem. Res. Chin. Univ.* **15**, 1807–1809.
Jin, L.-F. & Xiao, F.-P. (2005). *Acta Cryst.* E**61**, o1105–o1106.
Ma, Y.-Y., Yu, Y., Wu, Y.-F., Xiao, F.-P. & Jin, L.-F. (2005). *Acta Cryst.* E**61**, o3497–o3499.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.