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# 4-Acetylanilinium chloride monohydrate

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.032
$wR$ factor = 0.070
Data-to-parameter ratio = 18.0

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



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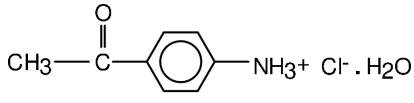
The crystal structure of the title compound, $C_8H_{10}NO^+\cdot Cl^-\cdot H_2O$, is composed of 4-acetylanilinium cations, chloride anions and water molecules of crystallization. The crystal packing features stacking interactions between the aromatic rings, with stacks running along the $c$ axis of the crystal, as well as extensive N—H···O, N—H···Cl and O—H···Cl hydrogen bonding which involves all five 'active' H atoms and links cations, anions and water molecules into a three-dimensional framework.

## Comment

The title salt, (I), is composed of 4-acetylanilinium ($C_8H_{10}NO^+$) cations, chloride anions and water molecules of crystallization. The cation is a protonated aniline derivative (Fig. 1); protonation results in a lengthening of the C1—N1 bond to 1.454 (2) Å. This bond is significantly longer than that in non-protonated anilines [1.335 (3) Å (Goswami *et al.*, 1999), 1.386 (4) Å (Ploug-Sørensen & Andersen, 1985) and 1.391 (3) Å (Ploug-Sørensen & Andersen, 1986)] and is typical for anilinium cations [1.464 (2) Å (Ploug-Sørensen & Andersen, 1985) and 1.460 (2) Å (Ploug-Sørensen & Andersen, 1986)].




(I)

The most significant feature of the crystal packing is the stack of aromatic rings running along the $c$ axis of the crystal; the distances between the centroids of neighbouring rings within the stack are 3.647 (2) and 3.648 (2) Å (Fig. 2). The chloride anions occupy the channels between the stacks.

All five 'active' H atoms in the structure are involved in hydrogen bonds of the N—H···O, O—H···Cl and N—H···Cl types (Table 2), linking all entities present in the structure into an infinite three-dimensional framework.

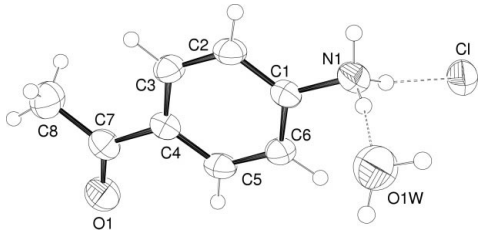



**Figure 1**
An *ORTEP*-3 (Farrugia, 1997) view of the cation, anion and water molecule in the structure of the title compound, showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. Hydrogen bonds are shown as dashed lines.

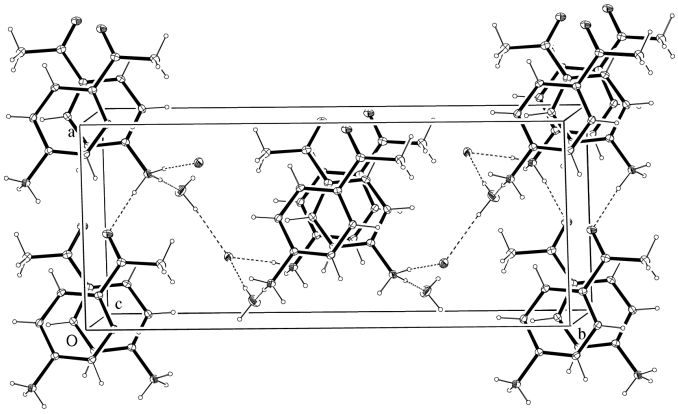



**Figure 2**
View of the packing of the title compound. Hydrogen bonds are shown as dashed lines.

## Experimental

The title compound, (I), was prepared by bubbling gaseous hydrogen chloride through a solution of 4-acetylaniline (2 g) in ether (50 ml) for 15 min at an approximate flow rate of 80 ml $min^{-1}$. The precipitate was filtered off and recrystallized from a mixture of ethanol and concentrated hydrochloric acid. The recrystallized product was dried in a desiccator, first over potassium hydroxide and then over phosphorus pentoxide.

*Crystal data*

$C_8H_{10}NO^+\cdot Cl^-\cdot H_2O$
$M_r$ = 189.64
Monoclinic, *Cc*
*a* = 7.690 (1) Å
*b* = 17.930 (1) Å
*c* = 7.095 (1) Å
$\beta$ = 95.70 (1)°
*V* = 973.4 (2) $Å^3$
*Z* = 4
$D_x$ = 1.294 Mg $m^{-3}$
Mo *K*$\alpha$ radiation
Cell parameters from 9241 reflections
$\theta$ = 2.3–28.9°
$\mu$ = 0.35 $mm^{-1}$
*T* = 293 (2) K
Prism, light yellow
0.30 × 0.21 × 0.21 mm

*Data collection*

Stoe IPDS-II diffractometer
$\omega$ scans
Absorption correction: numerical (*X-RED*32; Stoe & Cie, 2002)
$T_{min}$ = 0.915, $T_{max}$ = 0.928
7188 measured reflections
2447 independent reflections
2060 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051
$\theta_{max}$ = 28.9°
*h* = −10 → 10
*k* = −24 → 24
*l* = −9 → 9

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.070
*S* = 0.96
2447 reflections
136 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.28 e $Å^{-3}$
Absolute structure: Flack (1983), 1162 Friedel pairs
Flack parameter = 0.3 (2)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—N1 | 1.454 (2) | C7—O1 | 1.211 (2) |
| C2—C1—N1 | 119.4 (1) | O1—C7—C8 | 121.5 (2) |
| C6—C1—N1 | 118.74 (13) | C4—C7—C8 | 118.8 (2) |
| O1—C7—C4 | 119.7 (1) | | |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O1$^{i}$ | 0.89 | 1.94 | 2.826 (2) | 175 |
| O1*W*—H1*W*···Cl1$^{ii}$ | 0.85 (4) | 2.32 (4) | 3.147 (2) | 165 (3) |
| O1*W*—H2*W*···Cl1$^{iii}$ | 0.88 (3) | 2.21 (3) | 3.084 (2) | 174 (3) |
| N1—H1*B*···Cl1 | 0.89 | 2.21 | 3.089 (2) | 171 |
| N1—H1*C*···O1*W* | 0.89 | 1.81 | 2.697 (2) | 175 |

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

The aromatic and water H atoms were refined isotropically. In the aromatic ring, the refined C—H distances are in the range 0.92 (2)–0.98 (2) Å. In the water molecule, the O—H distances are 0.85 (4) and 0.88 (3) Å. The methyl and anilinium N-bound H atoms were included in the refinement in a riding-model approximation, with C—H = 0.96 Å, N—H = 0.89 Å and $U_{iso}$ = 1.5 $U_{eq}$(carrier atom).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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