# 4-Carboxyanilinium chloride

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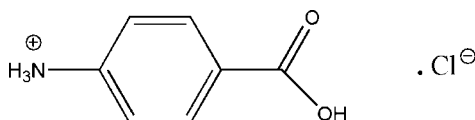
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In the title salt, $C_7H_8NO_2^+\cdot Cl^-$, the cation and anion are linked by an O—H$\cdots$Cl hydrogen bond. The three-dimensional crystal structure is stabilized by N—H$\cdots$O and N—H$\cdots$Cl hydrogen bonds.

## Related literature

For related structures, see: Athimoolam & Natarajan (2007); Gracin & Fischer (2005).



## Experimental

### Crystal data

| | |
|---|---|
| $C_7H_8NO_2^+\cdot Cl^-$ | $V$ = 787.9 (9) Å³ |
| $M_r$ = 173.59 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a$ = 5.601 (5) Å | $\mu$ = 0.43 mm⁻¹ |
| $b$ = 8.269 (5) Å | $T$ = 298 K |
| $c$ = 17.118 (5) Å | 0.50 × 0.40 × 0.30 mm |
| $\beta$ = 96.371 (5)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 4205 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2008) | 1299 independent reflections |
| $T_{min}$ = 0.814, $T_{max}$ = 0.882 | 1210 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.030 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.054 | 133 parameters |
| $wR(F^2)$ = 0.192 | All H-atom parameters refined |
| $S$ = 1.26 | $\Delta\rho_{max}$ = 0.49 e Å⁻³ |
| 1299 reflections | $\Delta\rho_{min}$ = −0.34 e Å⁻³ |

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O1—H1$\cdots$Cl1 | 0.99 (8) | 2.10 (8) | 3.059 (4) | 164 (6) |
| N1—H1$A\cdots$Cl1[i] | 0.85 (6) | 2.33 (6) | 3.154 (6) | 165 (5) |
| N1—H1$B\cdots$O2[ii] | 0.88 (9) | 2.05 (8) | 2.823 (6) | 145 (7) |
| N1—H1$B\cdots$Cl1[iii] | 0.88 (9) | 2.70 (9) | 3.289 (5) | 125 (6) |
| N1—H1$C\cdots$Cl1[ii] | 0.96 (8) | 2.26 (8) | 3.215 (5) | 172 (6) |

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg & Berndt, 1999); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2458).

## References

Athimoolam, S. & Natarajan, S. (2007). Acta Cryst. C63, o514–o517.
Brandenburg, K. & Berndt, M. (1999). DIAMOND. Crystal Impact GbR, Bonn, Germany.
Bruker (2008). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
Gracin, S. & Fischer, A. (2005). Acta Cryst. E61, o1242–o1244.
Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.

**supplementary materials**

## 4-Carboxyanilinium chloride

### L.-J. Han, S.-P. Yang, X. Tao and Y.-F. Ma

### Comment

We intended to prepare a cerium(III) complex of *p*-aminobenzoic acid. However, we obtained crystals of the title salt, and we report here its crystal structure.

In the title salt, the asymmetric unit consists of one *p*-aminobenzoic acid cation and one chloride anion (Fig. 1).

The amine group is protonated and the C4—N1 bond length is 1.471 (7) Å. In the crystal structure of 4-carboxyanilinium(2*R*, 3*R*)-tartrate (Athimoolam & Natarajan, 2007) the amine group is also protonated and the values of the corresponding C—N bond lengths are 1.464 (6) Å and 1.476 (5) Å.

In the crystal structures of the α-polymorph of *p*-aminobenzoic acid (Athimoolam & Natarajan, 2007) and β-polymorph of *p*-aminobenzoic acid (Gracin & Fischer, 2005) the amino group is not protonated. For the α-polymorph the C—N distance is 1.372 (5) Å; for the β-polymorph the distance is 1.408 (3) Å.

The hydrogen bonds listed in Table 1 result in a crystal structure generated by inversion and glide symmetry (Fig. 2).

### Experimental

To a solution containing *p*-aminobenzoic acid (1.37 g, 10 mmol) in ethanol (30 ml), a solution of cerium(III) chloride (1.24 g, 5 mmol) in methanol (15 ml) was added with stirring for 2 h at 323 K, and then the solution was filtered. Colourless crystals suitable for X-ray crystal structure analysis were obtained from the filtered solution over a period of two weeks.

### Refinement

All H atoms were located in a difference Fourier map and refined freely; $Csp^2$—H = 0.87 (6) – 0.96 (5) Å, N—H = 0.85 (6) – 0.96 (8) Å and O—H = 0.99 (8) Å.

### Figures



Fig. 1. The asymmetric unit of the title structure. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.
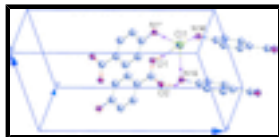


Fig. 2. Part of the crystal structure, with hydrogen bonds shown as dashed lines. For clarity, H atoms not involved in the hydrogen bonds have been omitted. [Symmetry code:(*).1 - *x*, 1 - *y*, 1 - *z* (#). 1 + *x*, 1/2 - *y*, 1/2 + *z*,(&). *x*, 1/2 - *y*, 1/2 + *z*].

# supplementary materials

## 4-Carboxyanilinium chloride

*Crystal data*

| | |
|---|---|
| $C_7H_8NO_2{}^+·Cl^-$ | $F(000) = 360$ |
| $M_r = 173.59$ | $D_x = 1.463$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 3678 reflections |
| $a = 5.601$ (5) Å | $\theta = 2.4$–$29.3°$ |
| $b = 8.269$ (5) Å | $\mu = 0.43$ mm$^{-1}$ |
| $c = 17.118$ (5) Å | $T = 298$ K |
| $\beta = 96.371$ (5)° | Block, yellow |
| $V = 787.9$ (9) Å$^3$ | $0.50 \times 0.40 \times 0.30$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 1299 independent reflections |
| Radiation source: fine-focus sealed tube | 1210 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.030$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | $h = -6 \rightarrow 6$ |
| $T_{min} = 0.814$, $T_{max} = 0.882$ | $k = -9 \rightarrow 7$ |
| 4205 measured reflections | $l = -20 \rightarrow 20$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.054$ | All H-atom parameters refined |
| $wR(F^2) = 0.192$ | $w = 1/[\sigma^2(F_o{}^2) + (0.0616P)^2 + 2.6608P]$ where $P = (F_o{}^2 + 2F_c{}^2)/3$ |
| $S = 1.26$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1299 reflections | $\Delta\rho_{max} = 0.49$ e Å$^{-3}$ |
| 133 parameters | $\Delta\rho_{min} = -0.34$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.075 (12) |

*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 ($Å^2$)*

|      | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|------|-----|-----|-----|-------------------|
| C1   | 0.5758 (9)  | 0.2824 (5)   | 0.5157 (3)   | 0.0322 (11) |
| C2   | 0.3637 (8)  | 0.1926 (6)   | 0.4999 (3)   | 0.0332 (11) |
| C3   | 0.3059 (9)  | 0.1230 (6)   | 0.4273 (3)   | 0.0367 (12) |
| C4   | 0.4607 (8)  | 0.1434 (5)   | 0.3701 (3)   | 0.0314 (11) |
| C5   | 0.6671 (9)  | 0.2347 (6)   | 0.3835 (3)   | 0.0362 (12) |
| C6   | 0.7245 (9)  | 0.3053 (6)   | 0.4564 (3)   | 0.0376 (12) |
| C7   | 0.6379 (9)  | 0.3487 (6)   | 0.5964 (3)   | 0.0348 (11) |
| N1   | 0.4043 (9)  | 0.0640 (6)   | 0.2933 (3)   | 0.0374 (10) |
| O1   | 0.8194 (7)  | 0.4512 (5)   | 0.6027 (2)   | 0.0488 (11) |
| O2   | 0.5313 (8)  | 0.3078 (5)   | 0.6508 (2)   | 0.0573 (12) |
| Cl1  | 0.9009 (2)  | 0.60977 (15) | 0.76491 (7)  | 0.0407 (5)  |
| H1   | 0.858 (13)  | 0.482 (9)    | 0.659 (5)    | 0.09 (2)*   |
| H1A  | 0.279 (10)  | 0.006 (6)    | 0.293 (3)    | 0.032 (14)* |
| H1B  | 0.393 (14)  | 0.131 (11)   | 0.253 (5)    | 0.09 (3)*   |
| H1C  | 0.545 (14)  | 0.002 (9)    | 0.286 (4)    | 0.08 (2)*   |
| H2   | 0.262 (9)   | 0.183 (6)    | 0.541 (3)    | 0.034 (13)* |
| H3   | 0.175 (10)  | 0.067 (6)    | 0.419 (3)    | 0.033 (13)* |
| H5   | 0.780 (10)  | 0.249 (6)    | 0.347 (3)    | 0.042 (15)* |
| H6   | 0.863 (9)   | 0.363 (6)    | 0.465 (3)    | 0.026 (12)* |

*Atomic displacement parameters ($Å^2$)*

|      | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|------|----------|----------|----------|----------|----------|----------|
| C1   | 0.035 (3) | 0.030 (2) | 0.033 (2) | 0.0025 (19) | 0.008 (2)  | 0.0034 (19) |
| C2   | 0.028 (2) | 0.039 (3) | 0.034 (2) | 0.001 (2)   | 0.008 (2)  | 0.006 (2)   |
| C3   | 0.033 (3) | 0.035 (3) | 0.045 (3) | −0.004 (2)  | 0.013 (2)  | 0.003 (2)   |
| C4   | 0.033 (2) | 0.028 (2) | 0.035 (2) | 0.0035 (19) | 0.009 (2)  | 0.0035 (18) |
| C5   | 0.035 (3) | 0.040 (3) | 0.036 (3) | 0.000 (2)   | 0.013 (2)  | 0.005 (2)   |
| C6   | 0.033 (3) | 0.037 (3) | 0.046 (3) | −0.007 (2)  | 0.015 (2)  | −0.001 (2)  |
| C7   | 0.031 (2) | 0.038 (2) | 0.034 (2) | 0.002 (2)   | 0.002 (2)  | 0.003 (2)   |
| N1   | 0.036 (2) | 0.041 (2) | 0.035 (2) | −0.004 (2)  | 0.006 (2)  | 0.0016 (19) |
| O1   | 0.054 (2) | 0.054 (2) | 0.039 (2) | −0.0211 (19)| 0.0078 (19)| −0.0046 (17)|

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.059 (3) | 0.080 (3) | 0.035 (2) | −0.025 (2) | 0.014 (2) | −0.0088 (19) |
| Cl1 | 0.0353 (8) | 0.0408 (8) | 0.0459 (8) | 0.0035 (5) | 0.0043 (5) | −0.0016 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.395 (6) | C5—C6 | 1.383 (7) |
| C1—C2 | 1.402 (7) | C5—H5 | 0.94 (5) |
| C1—C7 | 1.491 (7) | C6—H6 | 0.91 (5) |
| C2—C3 | 1.374 (7) | C7—O2 | 1.209 (6) |
| C2—H2 | 0.96 (5) | C7—O1 | 1.319 (6) |
| C3—C4 | 1.389 (6) | N1—H1A | 0.85 (6) |
| C3—H3 | 0.87 (6) | N1—H1B | 0.88 (9) |
| C4—C5 | 1.378 (7) | N1—H1C | 0.96 (8) |
| C4—N1 | 1.471 (7) | O1—H1 | 0.99 (8) |
| | | | |
| C6—C1—C2 | 119.6 (5) | C6—C5—H5 | 116 (3) |
| C6—C1—C7 | 121.8 (5) | C5—C6—C1 | 120.1 (5) |
| C2—C1—C7 | 118.6 (4) | C5—C6—H6 | 118 (3) |
| C3—C2—C1 | 120.4 (4) | C1—C6—H6 | 121 (3) |
| C3—C2—H2 | 122 (3) | O2—C7—O1 | 124.0 (5) |
| C1—C2—H2 | 117 (3) | O2—C7—C1 | 121.8 (5) |
| C2—C3—C4 | 119.0 (5) | O1—C7—C1 | 114.2 (4) |
| C2—C3—H3 | 118 (3) | C4—N1—H1A | 111 (3) |
| C4—C3—H3 | 123 (3) | C4—N1—H1B | 114 (5) |
| C5—C4—C3 | 121.7 (5) | H1A—N1—H1B | 111 (6) |
| C5—C4—N1 | 119.1 (4) | C4—N1—H1C | 104 (5) |
| C3—C4—N1 | 119.1 (4) | H1A—N1—H1C | 113 (6) |
| C4—C5—C6 | 119.3 (4) | H1B—N1—H1C | 103 (6) |
| C4—C5—H5 | 125 (3) | C7—O1—H1 | 109 (4) |
| | | | |
| C6—C1—C2—C3 | 2.1 (7) | C4—C5—C6—C1 | 0.7 (8) |
| C7—C1—C2—C3 | −176.9 (4) | C2—C1—C6—C5 | −2.3 (7) |
| C1—C2—C3—C4 | −0.1 (7) | C7—C1—C6—C5 | 176.6 (5) |
| C2—C3—C4—C5 | −1.6 (7) | C6—C1—C7—O2 | −167.9 (5) |
| C2—C3—C4—N1 | 177.7 (4) | C2—C1—C7—O2 | 11.1 (7) |
| C3—C4—C5—C6 | 1.4 (7) | C6—C1—C7—O1 | 10.8 (7) |
| N1—C4—C5—C6 | −177.9 (5) | C2—C1—C7—O1 | −170.2 (4) |

*Hydrogen-bond geometry (Å, °)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| O1—H1···Cl1 | 0.99 (8) | 2.10 (8) | 3.059 (4) | 164 (6) |
| N1—H1A···Cl1[i] | 0.85 (6) | 2.33 (6) | 3.154 (6) | 165 (5) |
| N1—H1B···O2[ii] | 0.88 (9) | 2.05 (8) | 2.823 (6) | 145 (7) |
| N1—H1B···Cl1[iii] | 0.88 (9) | 2.70 (9) | 3.289 (5) | 125 (6) |
| N1—H1C···Cl1[ii] | 0.96 (8) | 2.26 (8) | 3.215 (5) | 172 (6) |

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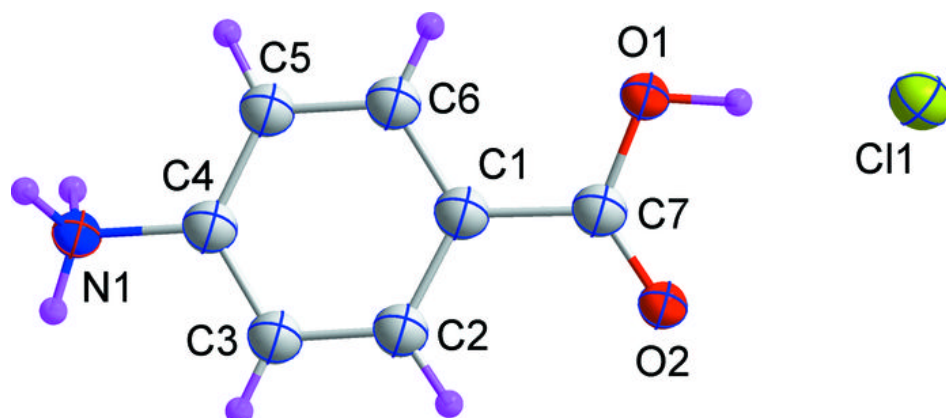
**Fig. 1**

**Fig. 2**