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7,8,9,10-Tetrahydro-11*H*-pyrido[2,3-*a*]carbazol-1-ium chloride

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Key indicators

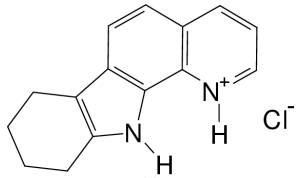
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.105
Data-to-parameter ratio = 16.8

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

The title compound, $C_{15}H_{15}N_2^+\cdot Cl^-$, (I), comprises the hydrochloride of an essentially planar tetracyclic molecule, which is protonated on the pyridine N atom. The Cl^- anion resides in the plane of the molecule and is bound by N—H···Cl interactions from both heterocyclic NH groups.

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis and was recrystallized from dilute HCl solution.



(I)

Crystal data

$C_{15}H_{15}N_2^+\cdot Cl^-$
M_r = 258.74
Monoclinic, $P2_1/c$
a = 15.9111 (6) Å
b = 5.0374 (2) Å
c = 17.1233 (9) Å
β = 113.9330 (17)°
V = 1254.44 (10) Å^3
Z = 4
D_x = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3819 reflections
θ = 2.9–27.5°
μ = 0.29 mm^{-1}
T = 150 (2) K
Needle, orange
0.35 × 0.07 × 0.06 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.906, T_{max} = 0.983
8962 measured reflections
2868 independent reflections
1761 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 27.5°
$h = -20 \rightarrow 18$
$k = -5 \rightarrow 6$
$l = -18 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.105
S = 0.99
2868 reflections
171 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1	1.01 (2)	2.03 (2)	3.038 (2)	175.7 (18)
N11—H11···Cl1	0.83 (2)	2.42 (2)	3.1880 (19)	155.2 (19)

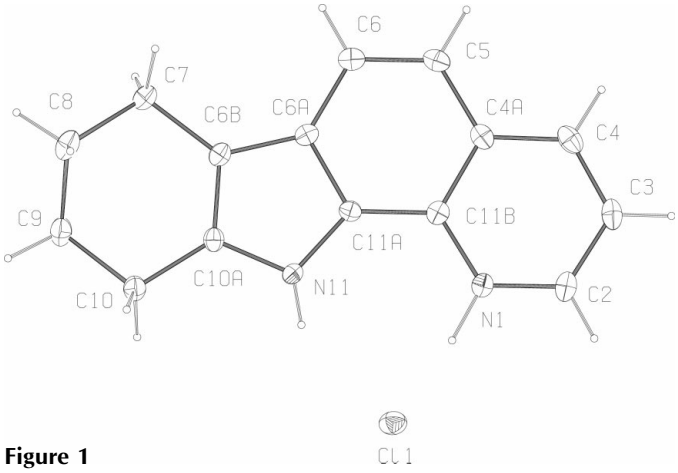


Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 30% probability ellipsoids.

All H atoms were included in the refinement at calculated positions as riding models, with C—H set to 0.95 (Ar-H) and 0.99 Å (CH_2), except for the N—H atoms, which were 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: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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