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8-Hydrazinoquinoline dihydrochloride hydrate

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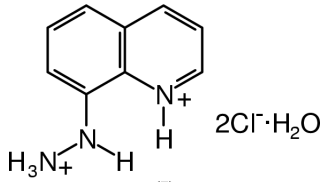
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.104
Data-to-parameter ratio = 15.0

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, $C_9H_{11}N_3{\cdot}2Cl{\cdot}H_2O$, comprises a planar cation containing two quaternary N atoms, packed in the solid-state with two Cl^- anions and one water molecule. Each component is involved in the hydrogen-bonding network, with one Cl^- anion and the O atom both being involved in three-centre associations, while the second Cl^- anion is involved in a four-centre association.



(I)

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from ethanol solution.

Crystal data

$C_9H_{11}N_3^{+}{\cdot}2Cl^{-}{\cdot}H_2O$
M_r = 250.12
Triclinic, $P\overline{1}$
a = 6.9716 (14) Å
b = 8.9866 (18) Å
c = 9.986 (2) Å
α = 70.04 (3)°
β = 89.20 (3)°
γ = 69.60 (3)°
V = 547.2 (3) Å^3
Z = 2
D_x = 1.518 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3835 reflections
θ = 2.9–27.5°
μ = 0.57 mm^{-1}
T = 150 (2) K
Plate, colourless
0.40 × 0.30 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.804, T_{max} = 0.945
7519 measured reflections
2465 independent reflections
2168 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
S = 1.04
2465 reflections
164 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2 + 0.1837P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1W^{i}	0.78 (2)	2.05 (2)	2.817 (2)	165 (2)
N81—H81···Cl1^{ii}	0.91 (2)	2.32 (2)	3.1983 (16)	164.5 (18)
N82—H82···Cl2^{ii}	0.91 (2)	2.25 (2)	3.1476 (18)	169.8 (18)
N82—H83···O1W^{iii}	0.87 (2)	1.94 (2)	2.808 (2)	178.7 (19)
N82—H84···Cl2^{iv}	0.89 (3)	2.39 (3)	3.1805 (17)	149.1 (19)
O1W—H1W···Cl1^{v}	0.84 (3)	2.21 (3)	3.0348 (17)	164 (2)
O1W—H2W···Cl2^{iii}	0.76 (3)	2.47 (3)	3.180 (2)	158 (2)

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

All aromatic H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.95 Å. All H atoms involved in the hydrogen-bonding network were located in difference syntheses and 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); molecular graphics: *PLATON*-97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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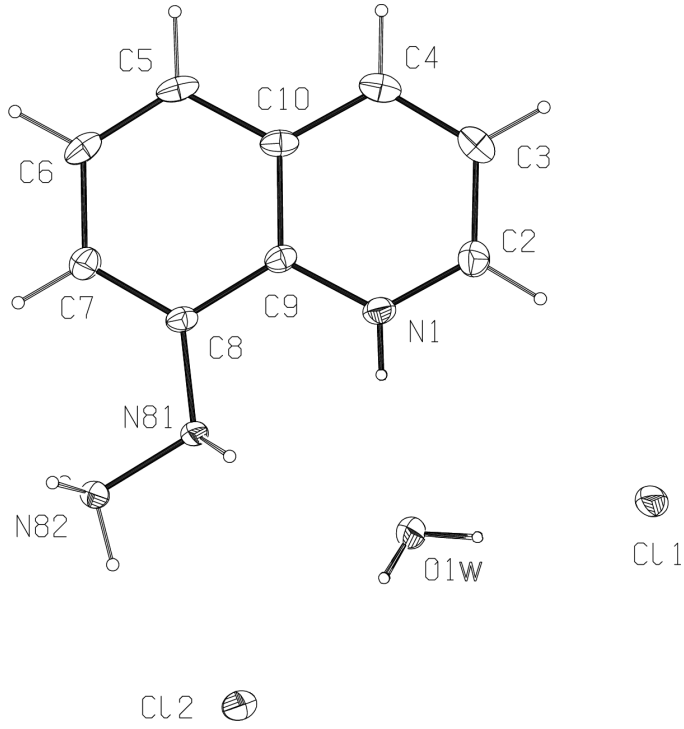

Figure 1
Molecular configuration and atom-numbering scheme for the title compound, showing 50% probability ellipsoids.

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