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Quinolinium perchlorate

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.108
Data-to-parameter ratio = 13.0

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

The crystal structure of the title compound, $C_9H_8N^+\cdot ClO_4^-$, consists of cations and anions linked by N—H···O and C—H···O hydrogen bonds to form layers parallel to the (102) plane.

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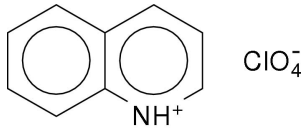
Comment

The title compound, (I), has previously been analysed using single-crystal X-ray photographic methods, but only the unit-cell dimensions and space group have been reported (Herbich & Lipkowski, 1975). The full structure determination of this compound is reported here.



(I)

In (I), the asymmetric unit is composed of one quinolinium cation and one perchlorate anion (Fig. 1). The cations and anions form hydrogen-bonded layers, parallel to the (102) plane and are linked together by a network of N—H···O and weak C—H···O hydrogen bonds (Fig. 2). The range of the observed hydrogen-bond parameters (Table 2) agrees with those accepted for N—H···O (Jeffrey, 1997) and C—H···O bonds (Desiraju & Steiner, 1999). Examination of the struc-

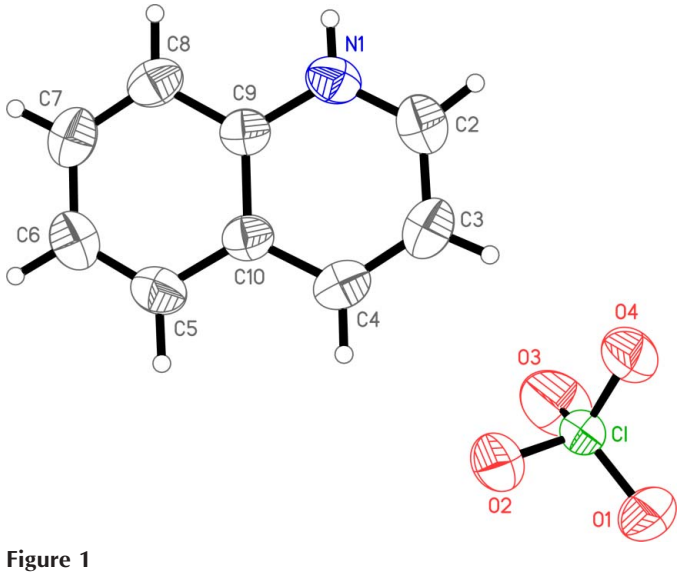


Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

ture with *PLATON* (Spek, 2003) reveals that parallel adjacent benzene rings are close together, with a perpendicular distance of 3.359 Å. However, a slippage of 2.426 Å and a distance between the ring centroids of 4.1434 (11) Å indicates no significant π–π stacking interactions between them.

The O atoms of the perchlorate anion are involved in different ways in the intermolecular hydrogen-bond system. An elongation of the Cl—O1 and Cl—O2 bond lengths [1.4400 (15) and 1.4377 (15) Å, respectively] caused by N—H···O bonds, in comparison with the remaining Cl—O3 and Cl—O4 bonds [1.4134 (18) and 1.4179 (15) Å, respectively], which are involved only in C—H···O interactions, is observed.

Experimental

The title compound was prepared by reaction of stoichiometric amounts of quinoline and perchloric acid (65%). The resulting solid was recrystallized from water.

Crystal data

$C_9H_8N^+\cdot ClO_4^-$
M_r = 229.61
Monoclinic, $P2_1/c$
a = 5.4935 (5) Å
b = 22.3315 (10) Å
c = 7.9970 (4) Å
β = 99.401 (6)°
V = 967.88 (11) Å^3
Z = 4
D_x = 1.576 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7554 reflections
θ = 1.8–30.3°
μ = 0.39 mm^{-1}
T = 291 K
Prism, colourless
0.6 × 0.3 × 0.2 mm

Data collection

Kuma KM-4 CCD diffractometer
ω scans
Absorption correction: none
8865 measured reflections
2190 independent reflections
1921 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°
$h = -5 \rightarrow 7$
$k = -28 \rightarrow 28$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.03
2190 reflections
169 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.3838P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.030 (3)

Table 1
Selected geometric parameters (Å, °).

Cl—O1	1.4400 (15)	C4—C10	1.414 (3)
Cl—O2	1.4377 (15)	C5—C6	1.360 (3)
Cl—O3	1.4134 (18)	C5—C10	1.413 (3)
Cl—O4	1.4179 (15)	C6—C7	1.402 (3)
N1—C2	1.324 (3)	C7—C8	1.361 (3)
N1—C9	1.371 (2)	C8—C9	1.407 (3)
C2—C3	1.378 (3)	C9—C10	1.415 (2)
C3—C4	1.366 (3)		
O1—Cl—O2	107.55 (9)	O2—Cl—O4	109.75 (10)
O1—Cl—O3	110.68 (12)	O3—Cl—O4	109.74 (11)
O1—Cl—O4	109.77 (10)	C2—N1—C9	123.12 (17)
O2—Cl—O3	109.31 (12)		

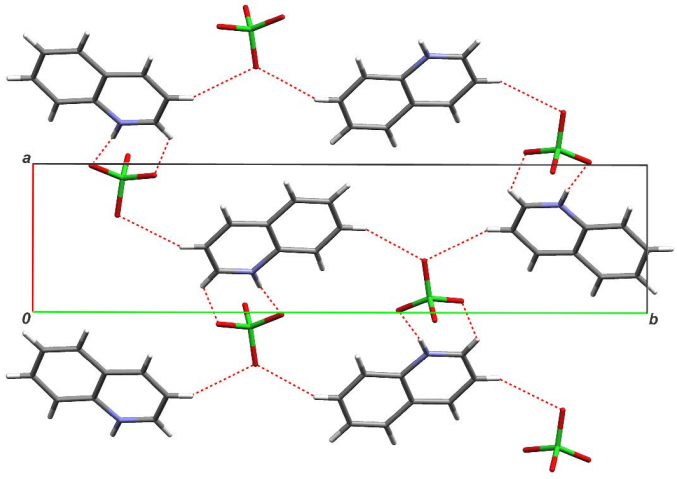


Figure 2
Packing diagram showing one layer of hydrogen-bonded (dashed lines) cations and anions parallel to the (102) plane, projected along the *c* axis.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.83 (2)	2.13 (2)	2.958 (2)	172 (2)
N1—H1···O2^{i}	0.83 (2)	2.59 (2)	3.156 (2)	127 (2)
C2—H2···O2^{i}	0.89 (2)	2.58 (2)	3.200 (3)	128 (2)
C5—H5···O3^{ii}	0.98 (2)	2.62 (2)	3.550 (3)	158 (2)
C7—H7···O4^{iii}	0.89 (2)	2.57 (2)	3.395 (3)	154 (2)

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

All H atoms were located in a difference map, and their coordinates and atomic displacement parameters were refined freely [C—H = 0.88 (3)–0.98 (2) Å].

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *MERCURY* (Version 1.3; Bruno *et al.*, 2002); software used to prepare material for publication: *PLATON* (Spek, 2003).

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