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7-Chloro-2,4-dimethyl-1,8-naphthyridin-1-ium nitrate

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Key indicators

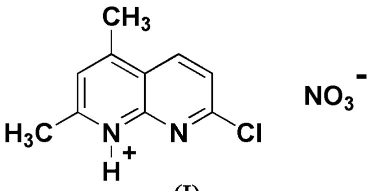
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.145
Data-to-parameter ratio = 12.9

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

In the title compound, $C_{10}H_{10}ClN_2^+\cdot NO_3^-$, the naphthyridinium cations and nitrate anions form cation–anion pairs *via* a strong N—H···O hydrogen bond.

Comment

The deriatives of 1,8-naphthyridine have been widely utilized in biochemistry and related fields. They can act as mono-dinucleating ligands (Gavrilova & Bosnich, 2004) for the preparation of multinuclear complexes, as molecular recognition receptors for urea, carboxylic acids and guanine (Goswami & Mukherjee, 1997; Nakatani *et al.*, 2000), as medicines (Stuk *et al.*, 2003; Ferrarini *et al.*, 2004), and as antimycobacterial and antimicrobial agents (Badawneh *et al.*, 2002; Badawneh *et al.*, 2003). Recently, 1,8-naphthyridine derivatives have been reported to be excellent fluorescent markers of nucleic acids (Hoock *et al.*, 1999) and probe molecules (Nakatani *et al.*, 2001). We report here the structure of the title compound, (I).



(I)

The molecules of (I) crystallize as positively charged ions with one N atom of the naphthyridine rings protonated, together with nitrate anions. The structure is shown in Fig. 1. The bond distances and angles are given in Table 1. The two methyl C atoms and the Cl atom are coplanar with the naphthyridine ring.

The naphthyridinium cations are connected by a strong N—H···O hydrogen bond to the nitrate anion (Table 2), forming cation–anion pairs.

Experimental

7-Chloro-2,4-dimethyl-1,8-naphthyridine was prepared according to a published procedure (Mangini & Colonna, 1943). The nitrate salt was prepared by adding 7-chloro-2,4-dimethyl-1,8-naphthyridine (19.2 mg) to concentrated nitric acid (0.1 ml) in water (3 ml). Upon slow evaporation of the solvent, colorless block crystals were obtained. Analysis calculated for $C_{10}H_{10}ClN_3O_3$: C 46.98, H 3.94, N 16.44%; found: C 46.77, H 4.18, N 16.29%.

Crystal data

$C_{10}H_{10}ClN_2^+ \cdot NO_3^-$
$M_r = 255.66$
Monoclinic, $P2_1/n$
$a = 9.477$ (5) Å
$b = 7.592$ (4) Å
$c = 16.017$ (9) Å
$\beta = 98.462$ (8)°
$V = 1139.9$ (11) Å^3
$Z = 4$
$D_x = 1.490$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.34$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.58 × 0.50 × 0.41 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.829$, $T_{max} = 0.875$
5723 measured reflections
2002 independent reflections
1505 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.145$
$S = 1.03$
2002 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 1.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.023 (3)

Table 1
Selected geometric parameters (Å, °).

Cl1—C2	1.735 (3)	C3—C4	1.357 (4)
N1—C8	1.324 (3)	C4—C5	1.416 (4)
N1—C1	1.363 (3)	C5—C6	1.426 (4)
N2—C2	1.299 (4)	C6—C7	1.366 (4)
N2—C1	1.352 (3)	C6—C9	1.497 (4)
C1—C5	1.405 (4)	C7—C8	1.400 (4)
C2—C3	1.401 (4)	C8—C10	1.489 (4)
C8—N1—C1	122.5 (2)	C1—C5—C4	116.2 (2)
C2—N2—C1	115.3 (2)	C1—C5—C6	118.4 (2)
N2—C1—N1	115.3 (2)	C4—C5—C6	125.4 (2)
N2—C1—C5	124.7 (2)	C7—C6—C5	118.1 (2)
N1—C1—C5	120.0 (2)	C7—C6—C9	120.9 (3)
N2—C2—C3	126.4 (3)	C5—C6—C9	121.0 (3)
N2—C2—Cl1	115.7 (2)	C6—C7—C8	121.9 (3)
C3—C2—Cl1	117.9 (2)	N1—C8—C7	119.0 (3)
C4—C3—C2	117.6 (3)	N1—C8—C10	118.1 (3)
C3—C4—C5	119.7 (3)	C7—C8—C10	122.9 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	1.84	2.700 (3)	176

All H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å, and N—H = 0.86 Å) and were allowed to ride on the atoms to which they are bonded, with $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3 groups and $U_{iso}(H) = 1.2U_{eq}$(C,N) for other H atoms.

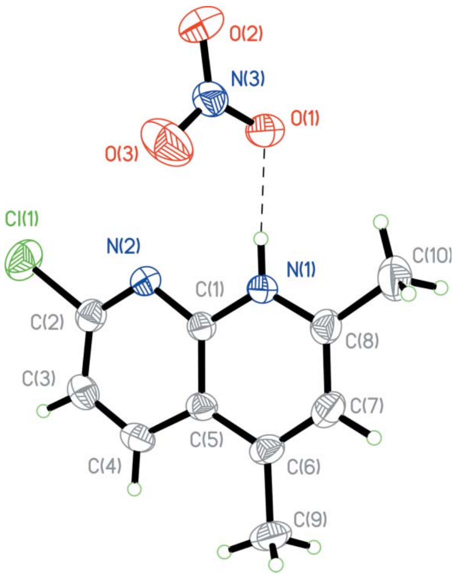


Figure 1
The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The dashed line indicates a hydrogen bond.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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