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A perchlorate salt of 1-[(2-dimethylaminoethylimino)methyl]naphthalen-2-ol

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
Disorder in solvent or counterion
R factor = 0.080
wR factor = 0.190
Data-to-parameter ratio = 11.7

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

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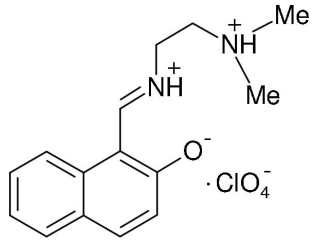
In the title compound, 1-[2-(dimethylammonio)ethyliminiomethyl]naphthalen-2-olate perchlorate, $C_{15}H_{19}N_2O^+\cdot ClO_4^-$, N—H···O hydrogen bonds link the ions into chains along the *a* axis. Adjacent chains are interlinked *via* C—H···O hydrogen bonds into layers parallel to the *ac* plane.

Comment

Compounds derived from 2-hydroxy-1-naphthaldehyde have been of great interest in coordination chemistry (Nishijima *et al.*, 1995; Zhao & Sun, 2005). We report here the crystal structure of one such compound, (I).



(I)

The bond lengths in (I) show normal values (Allen *et al.*, 1987). As expected, the molecule adopts a *trans* configuration with respect to the C11═N1 double bond. An intramolecular N1—H1···O5 hydrogen bond is observed in the molecular structure (Fig. 1). The cations are linked into chains *via* N2—H2*A*···O5($x-1$, y, z) hydrogen bonds along the *a* axis. The chains are interlinked into layers parallel to the *ac* plane by C—H···O hydrogen bonds involving the perchlorate O atoms (Fig. 2 and Table 1).

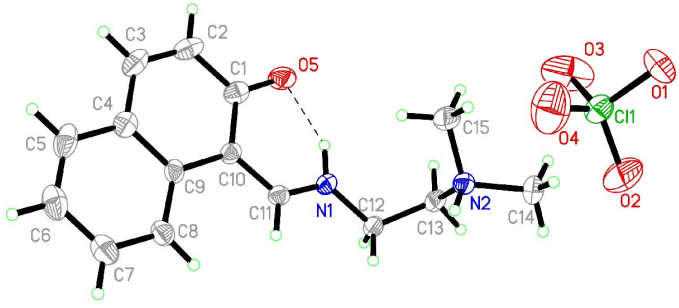


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only the major component of the disordered perchloate anion is shown. The intramolecular hydrogen bond is indicated by a dashed line.

Experimental

2-Hydroxy-1-naphthaldehyde (0.2 mmol, 17.2 mg) and *N*,*N*-dimethylethane-1,2-diamine (0.2 mmol, 17.6 mg) were dissolved in ethanol (10 ml). The mixture was stirred for 15 min to give a clear yellow solution. To this solution was added an aqueous solution of $HClO_4$ (0.2 mmol, 70%), with stirring. The mixture was stirred for 15 min at room temperature and filtered. The filtrate was allowed to stand in air for 12 d, after which time yellow block-shaped crystals formed on slow evaporation of the solvent.

Crystal data

$C_{15}H_{19}N_2O^+\cdot ClO_4^-$
M_r = 342.77
Monoclinic, $P2_1/n$
a = 6.126 (2) Å
b = 8.405 (2) Å
c = 30.985 (5) Å
β = 92.275 (3)°
V = 1594.1 (7) Å^3
Z = 4
D_x = 1.428 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1287 reflections
θ = 2.5–22.4°
μ = 0.27 mm^{-1}
T = 295 (2) K
Block, yellow
0.28 × 0.23 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.929, T_{max} = 0.946
11 554 measured reflections
2960 independent reflections
2030 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 25.5°
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -37 \rightarrow 37$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.190
S = 1.10
2960 reflections
253 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 1.812P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O5^{i}	0.90 (1)	1.79 (2)	2.670 (5)	168 (5)
N1—H1···O5	0.90 (1)	1.76 (3)	2.564 (5)	147 (5)
C5—H5A···O4^{ii}	0.93	2.56	3.395 (10)	150
C14—H14C···O3^{iii}	0.96	2.36	3.301 (12)	165
C15—H15B···O3	0.96	2.50	3.393 (9)	155

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

Atoms H1 and H2*A* were located in a difference Fourier map and refined isotropically, with the N—H distances restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). The O atoms of the perchlorate anion are disordered over two distinct sites with occupancies of 0.613 (12) and 0.387 (12). The Cl—O and O···O distances in both disordered components were restrained to be equal. The U^{ij} components of atoms O2, O4, O1′, O3′ and O4′ were restrained to isotropic behaviour.

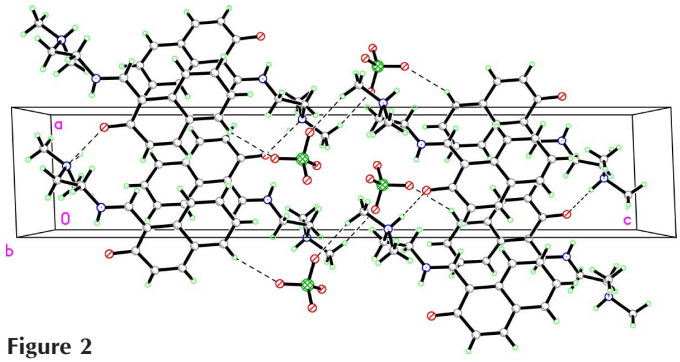


Figure 2
The crystal packing of (I), viewed along the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. Only the major disorder component is shown.

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

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