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Tetra-*n*-propylammonium perchlorate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.108
Data-to-parameter ratio = 22.3

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

The crystallographic analysis of the title compound, $C_{12}H_{28}N^{+}\cdot ClO_4^{-}$, (I), shows that intermolecular C—H···O interactions stabilize the crystal structure. The compound is isomorphous with tetra-*n*-propylammonium iodide, whose structure has been described by Yoshida *et al.* [*Acta Cryst.* (1994). C**50**, 1758–1760].

Comment

The title compound, (I) (Fig. 1 and Table 1), is isomorphous with tetra-*n*-propylammoinum iodide (Yoshida *et al.*, 1994). As detailed in Table 2 and Fig. 2, intermolecular C—H···O interactions are found between the tetra-*n*-propylammonium cations and the perchlorate anions.

$$[(CH_3CH_2CH_2)_4N]^{+}\cdot[ClO_4]^{-}$$

(I)

Experimental

A methanol solution (100 ml) was prepared for electrochemical studies containing tetra-*n*-propylammonium iodide (3.13 mg, 0.01 mmol), sodium iodide (1.49 mg, 0.01 mmol) and silver perchlorate (2.07 mg, 0.01 mmol) as electrolytes. Colorless single crystals of (I) were obtained from the slow evaporation of this solution (m.p. 510–512 K; literature m.p. 513–515 K; Beilstein 4, II, 628). Analysis found: C 50.42, H 9.89, N 4.88%; calculated for $C_{12}H_{28}NO_4Cl$: C 50.43, H 9.87, N 4.90%. ^{1}H NMR (400 MHz, D_2O): δ 3.15 (8H, *m*, CH_2), 1.69 (8H, *m*, CH_2), 0.94 (12H, *t*, CH_3).

Crystal data

$C_{12}H_{28}N^{+}\cdot ClO_4^{-}$
M_r = 285.80
Orthorhombic, $P2_12_12_1$
a = 13.3335 (9) Å
b = 12.1528 (8) Å
c = 9.6210 (6) Å
V = 1558.98 (18) Å^3
Z = 4
D_x = 1.218 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 2126 reflections
θ = 2.3–21.6°
μ = 0.25 mm^{-1}
T = 173 (2) K
Needle, colorless
0.48 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.889, T_{max} = 0.951
11 458 measured reflections

3723 independent reflections
2851 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.9°
$h = -17 \rightarrow 14$
$k = -15 \rightarrow 15$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.108
S = 1.00
3723 reflections
167 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ <0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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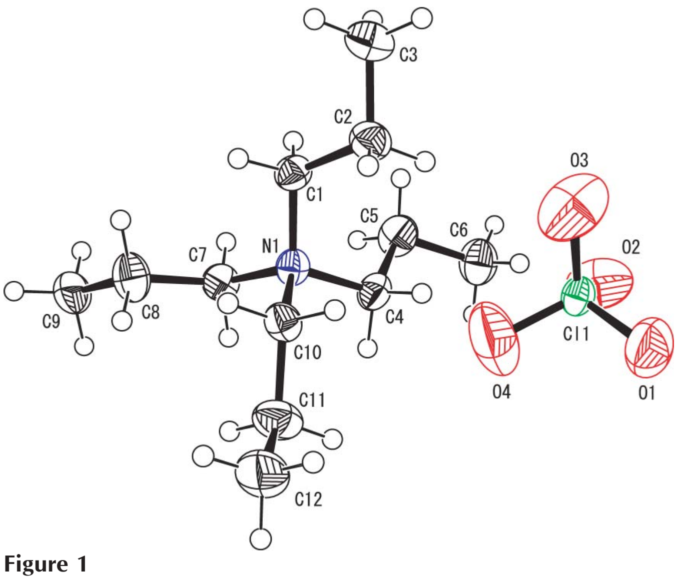

Figure 1
A perspective view of the title compound, with the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

Table 1
Selected interatomic distances (Å).

C1—N1	1.515 (3)	C7—C8	1.516 (4)
C1—C2	1.519 (4)	C7—N1	1.531 (3)
C2—C3	1.508 (4)	C8—C9	1.531 (3)
C4—C5	1.519 (4)	C10—C11	1.508 (3)
C4—N1	1.528 (3)	C10—N1	1.519 (3)
C5—C6	1.511 (4)	C11—C12	1.520 (4)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···O4	0.99	2.42	3.288 (3)	146
C7—H7*B*···O2^{i}	0.99	2.51	3.478 (3)	166
C6—H6*C*···O1^{i}	0.98	2.59	3.334 (4)	133
C5—H5*B*···O4^{ii}	0.99	2.58	3.423 (4)	143
C4—H4*A*···O4	0.99	2.60	3.500 (3)	152
C1—H1*A*···O3^{iii}	0.99	2.41	3.356 (4)	160

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

All H atoms were placed in calculated positions, with C—H = 0.99 (for CH_2) or 0.98 Å (for CH_3), and were refined in the riding-model approximation, with U_{iso}(H) = $1.2U_{eq}$(carrier atom). The highest residual electron density peak is associated with the perchlorate anion, indicative of some degree of orientational disorder, which was not modeled. The absolute structure could not be determined reliably and hence Friedel pairs were merged in the final refinement.

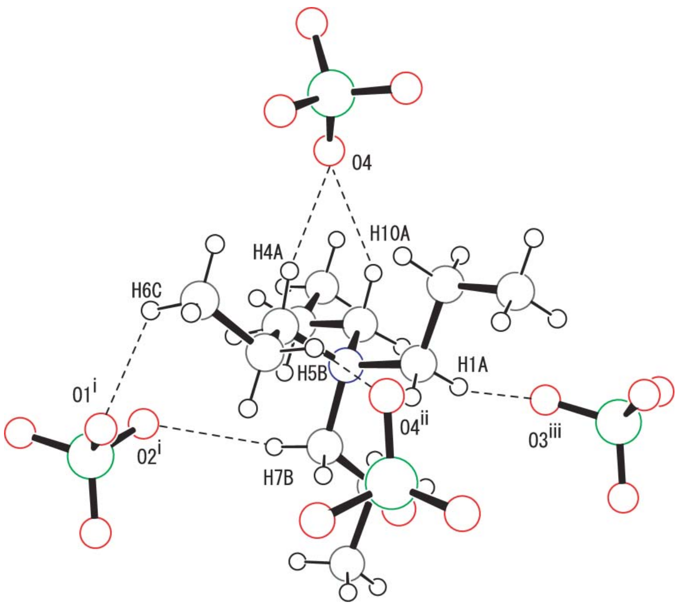

Figure 2
Diagram showing the intermolecular C—H···O interactions (dashed lines). [Symmetry codes: (i) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $-\frac{1}{2}+x, \frac{3}{2}-y, -z$; (iii) $1-x, \frac{1}{2}+y, -\frac{1}{2}-z$.]

Data collection: *SMART-W2K/NT* (Bruker, 2003); cell refinement: *SAINT-W2K/NT* (Bruker, 2003); data reduction: *SAINT-W2K/NT*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 2003); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL-NT*.

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