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R-(3-Carboxy-2-hydroxypropyl)trimethylazanium chloride

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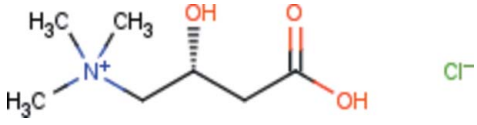
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.072; data-to-parameter ratio = 19.2.

In the title salt [common name L-carnitine hydrochloride], $C_7H_{16}NO_3^+\cdot Cl^-$, the organic cation features a carboxylic part (–CO_2H) having unambigous single- and double-bonds [1.336 (2), 1.211 (2) Å]. There is a large N—C—C bond angle [115.9 (1)°] for the C atom connected to the bulky trimethylamino substituent. In the crystal, the acid H atom forms a hydrogen bond to the chloride anion, whereas the hydroxyl H atom forms a longer hydrogen bond to the anion, generating a helical chain running along [001].

Related literature

For racemic carnitine hydrochloride, see: Tomita *et al.* (1974); Yunuskhodzhaev *et al.* (1991). For *R*-carnitine, see: Gandour *et al.* (1985).



Experimental

Crystal data

$C_7H_{16}NO_3^+\cdot Cl^-$
M_r = 197.66
Orthorhombic, $P2_12_12_1$
a = 6.3043 (3) Å
b = 11.5256 (7) Å
c = 13.4905 (8) Å
V = 980.23 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 100 K
0.40 × 0.30 × 0.20 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan *CrysAlis PRO* (Agilent, 2012)
T_{min} = 0.869, T_{max} = 0.931
6682 measured reflections
2251 independent reflections
2191 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.072
S = 1.09
2251 reflections
117 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 926 Friedel pairs
Flack parameter: 0.01 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Cl1	0.85 (1)	2.18 (1)	3.022 (1)	176 (2)
O3—H3···Cl1^{i}	0.83 (1)	2.51 (2)	3.209 (1)	142 (2)

Symmetry code: (i) $-x+\frac{1}{2}, -y, z-\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5512).

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supplementary materials

Acta Cryst. (2012). E**68**, o1416 [doi:10.1107/S160053681201598X]

(*R*)-(3-Carboxy-2-hydroxypropyl)trimethylazanium chloride

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Comment

A model for the binding of *L*-carnitine to the carnitine acetyltransferase enzyme has been proposed on the basis of the crystal structure of *L*-carnitine (Gandour *et al.*, 1985). *L*-Carnitine, a zwitterionic compound that is biosynthesized from lysine and methinonine, is the vitamin B_T; it is also avaliable commerically as the hydrochloride salt. The crystal structure of racemic carnitine hydrochloride has been previously reported (Tomita *et al.*, 1974; Yunuskhodzhaev *et al.*, 1991). In the crystal structure of *L*-carnitine hydrochloride (Scheme I), the carboxyl $–CO_2$ part carries the acid hydrogen (Fig. 1). This part has unambigous single- and double-bonds [1.336 (2), 1.211 (2) Å]. The three-atom $C_{carboxyl}$–*C*–$C_{trimethylamino}$ unit shows a large angle [115.9 (1) °] for the atom connected to the bulky trimethylamino substituent. The acid hydrogen forms a hydrogen bond to the chloride anion (Table 1). Oddly, the hydroxy group does not engage in any hydrogen bonding interactions.

Experimental

L-Carnithine hydrochloride as supplied by Sigma Chemical Company consists of colorless prismatic crystals, and was used without purification.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.98 to 1.00 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

The hydroxy and acid H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84±0.01 Å; their temperature factors were refined.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

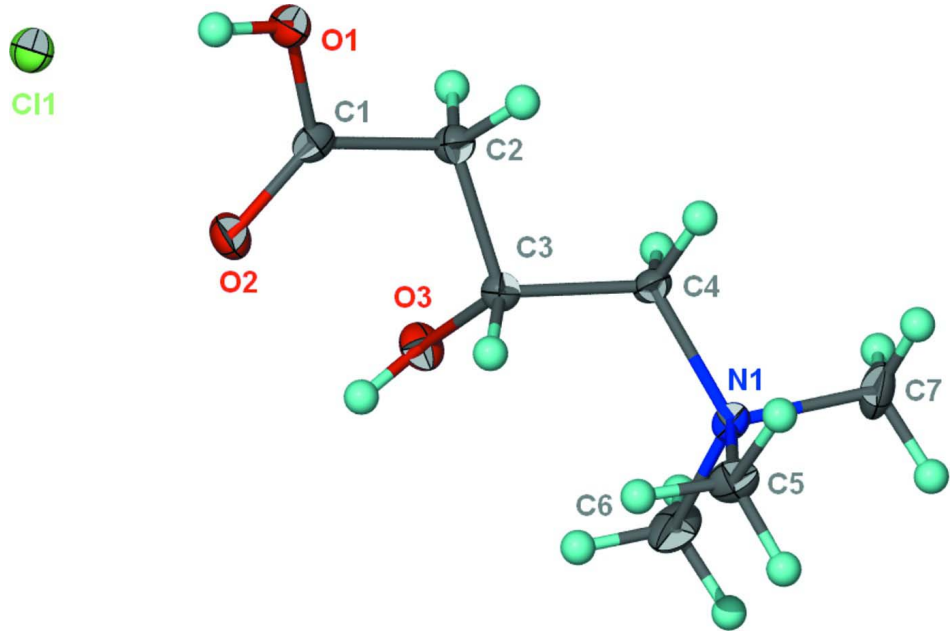

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_7H_{16}NO_3^+\cdot Cl^-$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

(*R*)-(3-Carboxy-2-hydroxypropyl)trimethylazanium chloride

Crystal data

$C_7H_{16}NO_3^+\cdot Cl^-$
$M_r = 197.66$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.3043\ (3)$ Å
$b = 11.5256\ (7)$ Å
$c = 13.4905\ (8)$ Å
$V = 980.23\ (10)$ Å^3
$Z = 4$

$F(000) = 424$
$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3837 reflections
$\theta = 2.3$–$27.5°$
$\mu = 0.36$ mm^{-1}
$T = 100$ K
Prism, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan *CrysAlis PRO* (Agilent, 2012)

$T_{min} = 0.869$, $T_{max} = 0.931$
6682 measured reflections
2251 independent reflections
2191 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -8\rightarrow8$
$k = -12\rightarrow15$
$l = -16\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.072$
$S = 1.09$
2251 reflections
117 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0381P)^2 + 0.129P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Absolute structure: Flack (1983), 926 Friedel pairs
Flack parameter: 0.01 (5)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.16829 (6)	−0.02923 (3)	1.11989 (3)	0.01599 (10)
O1	0.11377 (16)	0.20168 (9)	1.01683 (8)	0.0153 (2)
H1	0.123 (3)	0.1372 (11)	1.0468 (14)	0.032 (6)*
O2	0.09374 (17)	0.09692 (9)	0.87751 (9)	0.0164 (2)
O3	0.03544 (17)	0.23605 (10)	0.69856 (8)	0.0146 (2)
H3	0.066 (4)	0.1658 (10)	0.6948 (18)	0.047 (7)*
N1	0.38932 (18)	0.40990 (10)	0.62406 (10)	0.0107 (2)
C1	0.1083 (2)	0.19013 (12)	0.91830 (11)	0.0113 (3)
C2	0.1258 (2)	0.30406 (12)	0.86490 (11)	0.0120 (3)
H2A	0.2287	0.3542	0.9001	0.014*
H2B	−0.0138	0.3435	0.8659	0.014*
C3	0.1976 (2)	0.28843 (12)	0.75711 (10)	0.0103 (3)
H3A	0.3279	0.2390	0.7552	0.012*
C4	0.2485 (2)	0.40787 (13)	0.71538 (11)	0.0109 (3)
H4A	0.1132	0.4470	0.6989	0.013*
H4B	0.3182	0.4540	0.7680	0.013*
C5	0.6024 (2)	0.35642 (13)	0.64467 (12)	0.0151 (3)
H5A	0.6887	0.3582	0.5843	0.023*
H5B	0.5834	0.2758	0.6661	0.023*
H5C	0.6741	0.4003	0.6971	0.023*
C6	0.2902 (3)	0.35091 (15)	0.53684 (11)	0.0198 (4)
H6A	0.3867	0.3552	0.4800	0.030*
H6B	0.1563	0.3895	0.5203	0.030*
H6C	0.2628	0.2694	0.5531	0.030*
C7	0.4241 (3)	0.53502 (13)	0.59814 (12)	0.0187 (3)
H7A	0.5126	0.5402	0.5386	0.028*
H7B	0.4954	0.5742	0.6533	0.028*
H7C	0.2871	0.5723	0.5856	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02265 (18)	0.01262 (16)	0.01271 (18)	0.00108 (14)	0.00145 (14)	0.00228 (14)
O1	0.0237 (6)	0.0118 (5)	0.0104 (5)	0.0005 (5)	0.0008 (4)	0.0021 (4)

O2	0.0218 (5)	0.0124 (5)	0.0150 (5)	−0.0037 (4)	−0.0005 (5)	−0.0013 (4)
O3	0.0161 (5)	0.0142 (5)	0.0135 (6)	−0.0021 (5)	−0.0049 (4)	−0.0009 (4)
N1	0.0103 (6)	0.0117 (5)	0.0102 (6)	0.0002 (5)	0.0010 (5)	0.0014 (5)
C1	0.0073 (6)	0.0149 (7)	0.0118 (7)	0.0007 (6)	0.0006 (5)	0.0008 (6)
C2	0.0126 (7)	0.0121 (6)	0.0112 (7)	0.0013 (6)	0.0002 (5)	0.0003 (5)
C3	0.0095 (6)	0.0109 (6)	0.0106 (7)	0.0008 (5)	−0.0011 (5)	0.0004 (6)
C4	0.0114 (6)	0.0115 (6)	0.0099 (7)	0.0010 (6)	0.0024 (5)	0.0004 (6)
C5	0.0118 (7)	0.0180 (7)	0.0155 (8)	0.0044 (6)	0.0011 (6)	0.0008 (6)
C6	0.0210 (8)	0.0305 (9)	0.0081 (8)	−0.0080 (7)	−0.0022 (6)	−0.0002 (6)
C7	0.0167 (7)	0.0134 (7)	0.0260 (9)	−0.0003 (7)	0.0062 (6)	0.0078 (7)

Geometric parameters (Å, º)

O1—C1	1.3363 (18)	C3—C4	1.521 (2)
O1—H1	0.848 (9)	C3—H3A	1.0000
O2—C1	1.2105 (18)	C4—H4A	0.9900
O3—C3	1.4262 (18)	C4—H4B	0.9900
O3—H3	0.833 (9)	C5—H5A	0.9800
N1—C6	1.4956 (19)	C5—H5B	0.9800
N1—C7	1.5000 (19)	C5—H5C	0.9800
N1—C5	1.5042 (18)	C6—H6A	0.9800
N1—C4	1.5188 (18)	C6—H6B	0.9800
C1—C2	1.5018 (19)	C6—H6C	0.9800
C2—C3	1.534 (2)	C7—H7A	0.9800
C2—H2A	0.9900	C7—H7B	0.9800
C2—H2B	0.9900	C7—H7C	0.9800
C1—O1—H1	112.9 (14)	N1—C4—H4A	108.3
C3—O3—H3	106.3 (18)	C3—C4—H4A	108.3
C6—N1—C7	108.35 (12)	N1—C4—H4B	108.3
C6—N1—C5	109.41 (12)	C3—C4—H4B	108.3
C7—N1—C5	107.84 (12)	H4A—C4—H4B	107.4
C6—N1—C4	112.76 (11)	N1—C5—H5A	109.5
C7—N1—C4	106.82 (11)	N1—C5—H5B	109.5
C5—N1—C4	111.47 (11)	H5A—C5—H5B	109.5
O2—C1—O1	122.86 (14)	N1—C5—H5C	109.5
O2—C1—C2	124.29 (14)	H5A—C5—H5C	109.5
O1—C1—C2	112.83 (12)	H5B—C5—H5C	109.5
C1—C2—C3	111.95 (11)	N1—C6—H6A	109.5
C1—C2—H2A	109.2	N1—C6—H6B	109.5
C3—C2—H2A	109.2	H6A—C6—H6B	109.5
C1—C2—H2B	109.2	N1—C6—H6C	109.5
C3—C2—H2B	109.2	H6A—C6—H6C	109.5
H2A—C2—H2B	107.9	H6B—C6—H6C	109.5
O3—C3—C4	109.21 (11)	N1—C7—H7A	109.5
O3—C3—C2	111.29 (11)	N1—C7—H7B	109.5
C4—C3—C2	107.87 (11)	H7A—C7—H7B	109.5
O3—C3—H3A	109.5	N1—C7—H7C	109.5
C4—C3—H3A	109.5	H7A—C7—H7C	109.5
C2—C3—H3A	109.5	H7B—C7—H7C	109.5

N1—C4—C3	115.93 (12)		
O2—C1—C2—C3	−19.23 (19)	C7—N1—C4—C3	−178.16 (13)
O1—C1—C2—C3	159.77 (12)	C5—N1—C4—C3	−60.59 (16)
C1—C2—C3—O3	70.19 (14)	O3—C3—C4—N1	−78.63 (15)
C1—C2—C3—C4	−170.02 (12)	C2—C3—C4—N1	160.28 (11)
C6—N1—C4—C3	62.93 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···Cl1	0.85 (1)	2.18 (1)	3.022 (1)	176 (2)
O3—H3···Cl1^{i}	0.83 (1)	2.51 (2)	3.209 (1)	142 (2)

Symmetry code: (i) −*x*+1/2, −*y*, *z*−1/2.