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Bis(ethylammonium) (–)-(2*S*,3*S*)-tartrate monohydrate

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Key indicators

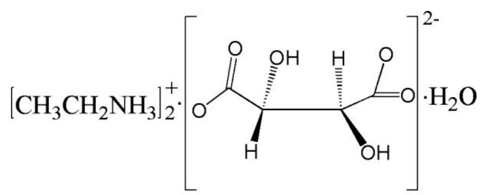
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.109
Data-to-parameter ratio = 9.8

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

The asymmetric unit of the title salt, $2C_2H_8N^+\cdot C_4H_4O_6^-\cdot H_2O$, contains two ethylammonium cations, one (2*S*,3*S*)-(−)-tartrate anion and one water molecule, which are linked by intermolecular N—H···O and O—H···O hydrogen bonds, leading to an infinite three-dimensional framework. An intramolecular hydrogen bond influences the structure of the (2*S*,3*S*)-(−)-tartrate anion.

Comment

In recent years, tartaric acid has been used as a polyfunctional ligand to build novel complexes with transition or alkaline-earth metals (Torres *et al.*, 2002; Lu *et al.*, 2005). However, to the best of our knowledge, there are few structures reported in which tartrate interacts with organic bases through hydrogen bonds to form supramolecular assemblies (Marchewka *et al.*, 2003). We report here the structure of the title salt, (I).



(I)

The asymmetric unit of (I) contains one (2*S*,3*S*)-(−)-tartrate anion, two singly protonated ethylammonium cations and one water molecule (Fig. 1). These ions and the solvent water molecule are linked by intermolecular N—H···O and O—H···O hydrogen bonds (Fig. 2 and Table 1) into an infinite three-dimensional framework (Fig. 3). An intramolecular hydrogen bond influences the structure of the tartrate anion.

Experimental

(2*S*,3*S*)-Tartaric acid (1 mmol, 0.150 g) was dissolved in 15 ml ethylamine and 5 ml distilled water. The mixture was stirred for 30 min at room temperature. The solution was filtered, and the filtrate was left to stand at room temperature. Colourless crystals of (I) were obtained from the filtrate after 6 d.

Crystal data

$2C_2H_8N^+\cdot C_4H_4O_6^-\cdot H_2O$	Z = 4
M_r = 258.28	D_x = 1.272 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
a = 6.9983 (12) Å	μ = 0.11 mm^{-1}
b = 8.0652 (14) Å	T = 293 (2) K
c = 23.898 (4) Å	Block, colourless
V = 1348.9 (4) Å^3	0.40 × 0.36 × 0.30 mm

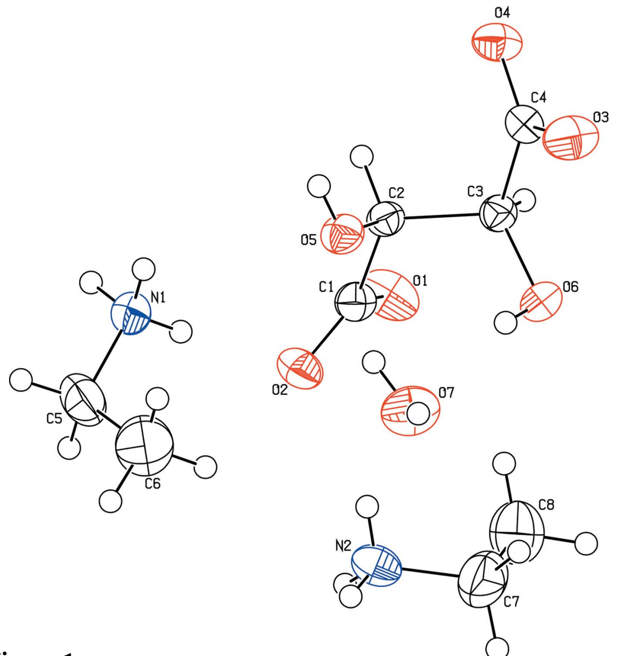


Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

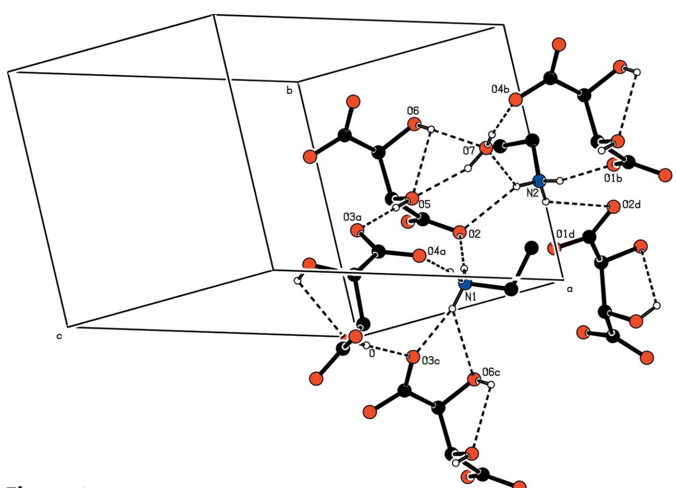


Figure 2
Part of the crystal structure of (I). H atoms not involved in hydrogen bonds have been omitted for clarity. Hydrogen bonds are shown as dashed lines. [Symmetry codes: (*a*) $1 - x, -\frac{1}{2} + y, \frac{1}{2} - z$; (*b*) $1 + x, y, z$; (*c*) $x, -1 + y, z$; (*d*) $\frac{1}{2} + x, \frac{1}{2} - y, -z$.]

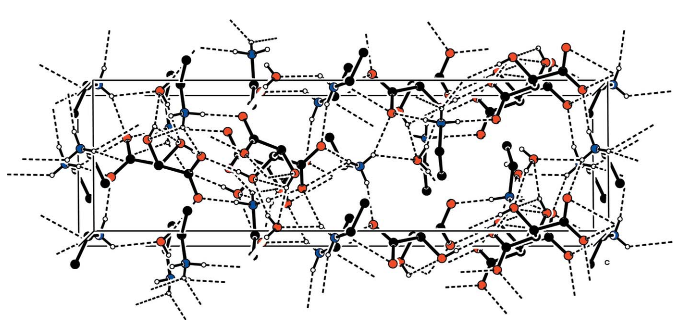


Figure 3
Packing of (I) viewed along the *b* axis. For clarity, H atoms not involved in hydrogen bonds have been omitted. Hydrogen bonds are shown as dashed lines.

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\rm min} = 0.957$, $T_{\rm max} = 0.968$

8607 measured reflections
1901 independent reflections
1774 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.131$
$\theta_{\rm max} = 28.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.109$
$S = 1.07$
1901 reflections
194 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2 + 0.1016P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.26$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.33$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2*C*$\cdots$O1$^{\rm i}$	0.85 (3)	1.97 (3)	2.792 (2)	161 (3)
N2—H2*B*$\cdots$O7	0.82 (3)	2.44 (3)	3.008 (2)	127 (2)
N2—H2*B*$\cdots$O2	0.82 (3)	2.25 (3)	2.959 (2)	146 (3)
N2—H2*A*$\cdots$O2$^{\rm ii}$	0.84 (3)	2.59 (3)	3.171 (2)	127 (3)
N2—H2*A*$\cdots$O1$^{\rm ii}$	0.84 (3)	2.00 (3)	2.835 (2)	172 (3)
N1—H1*C*$\cdots$O6$^{\rm iii}$	0.89 (3)	2.59 (3)	3.291 (2)	135 (2)
N1—H1*C*$\cdots$O3$^{\rm iii}$	0.89 (3)	1.99 (3)	2.793 (2)	149 (2)
N1—H1*B*$\cdots$O2	0.87 (4)	1.99 (4)	2.854 (2)	176 (3)
N1—H1*A*$\cdots$O4$^{\rm iv}$	0.89 (3)	1.90 (3)	2.790 (2)	172 (2)
O7—H7*B*$\cdots$O5	0.86 (4)	1.94 (4)	2.751 (2)	156 (3)
O7—H7*A*$\cdots$O4$^{\rm i}$	0.77 (3)	1.97 (3)	2.732 (2)	172 (3)
O6—H6$\cdots$O5	0.81 (3)	2.53 (3)	2.9440 (19)	113 (2)
O6—H6$\cdots$O7	0.81 (3)	2.07 (3)	2.851 (2)	163 (3)
O5—H5$\cdots$O3$^{\rm iv}$	0.76 (3)	1.92 (3)	2.6786 (19)	177 (3)

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

In the absence of significant anomalous dispersion effects, Friedel pairs were averaged. All H atoms bound to carbon were refined using a riding model, with C—H = 0.98 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) for CH, C—H = 0.97 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) for CH_2, and C—H = 0.96 Å and $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(C) for CH_3. Water H atoms were located in a difference map and refined with their O—H and H$\cdots$H distances restrained to 0.83 (1) and 1.34 (1) Å, respectively. Other H atoms bonded to N and O were located in a difference map and refined freely.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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