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Sarcosinium tartrate

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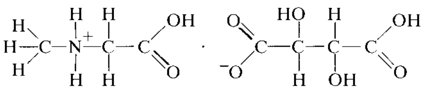
In the title compound, $C_3H_8NO_2^+\cdot C_4H_5O_6^-$, the sarcosinium cation and semi-tartrate anion are held together by a three-dimensional network of O—H···O, N—H···O and C—H···O hydrogen bonds. The structure may be described as an inclusion compound with the semi-tartrate anion as the host and the sarcosinium cation as the guest.

Comment

Single-crystal X-ray investigations on complexes of amino acids with carboxylic acids are interesting in view of their geometrical features and aggregation patterns that might possibly have occurred in prebiotic polymerization (Vijayan, 1988; Prasad & Vijayan, 1993). The present study reports the crystal structure of a complex, (I), of sarcosine with tartaric acid. Sarcosine (*N*-methylglycine, $CH_3NH_2^+CH_2COO^-$) is an α-amino acid present in several biologically important compounds and its crystal structure was elucidated in our laboratory (Mostad & Natarajan, 1989).



$$\mathrm{H_3C-N^+H_2-CH_2-C(=O)OH \cdot {}^-O(O=)C-CH(OH)-CH(OH)-C(=O)OH}$$

(I)

The sarcosine moiety exists in the cationic form with a positively charged amino group and a neutral carboxylic acid group. The C1—C2—N1—C3 chain deviates greatly from planarity as the torsion angle about the C2—N1 bond is −67.2 (2)°, indicating that the methyl group exists in the synclinal conformation with respect to C1.

The tartaric acid molecule (Okaya *et al.*, 1966) exists here as a semi-tartrate ion with a neutral carboxylic acid group and a negatively charged carboxylate ion. The C4—O3 and C4=O4 bond distances [1.288 (3) and 1.222 (3) Å, respectively] of the neutral carboxylic acid group are significantly different from those expected. The decrease in the C—O and increase in the C=O bond lengths may be attributed to a strong O3—H3···O7($x-1$, $y+1$, z) hydrogen bond observed in the crystal structure, with an O···O distance of 2.488 (2) Å. This observation is supported by the fact that strong O—H···*X* hydrogen bonds involving the carboxylic acid group O atom as donor permit some double-bond character to the C—O and some single-bond character to C=O (Hahn, 1957). The angle between the planes of the half molecules (O3/O4/C4/C5/O5 and O7/O8/C6/C7/O6) is 65.10 (7)°, which is somewhat larger than the value of 54.6 (4)° found in the structure of tartaric acid. The carbon skeleton of the semi-tartrate anion is essentially planar [torsion angle C4—C5—C6—C7 of 179.21 (15)°].

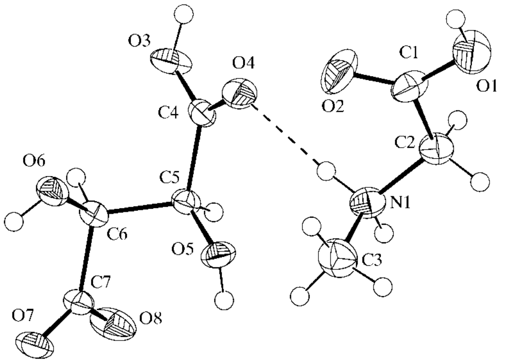


Figure 1
The molecular structure of (I) with the atom-numbering scheme and 50% probability displacement ellipsoids.

The crystal structure (Fig. 2) is stabilized by hydrogen bonds (Table 1). The semi-tartrate ions aggregate into layers parallel to the *ab* plane. The layers are interconnected by sarcosinium cations which do not directly interact among themselves, except for the presence of a weak C—H···O hydrogen bond. The crystal structure can be described as an inclusion compound with the semi-tartrate anion as the host and the sarcosinium cation as the guest.

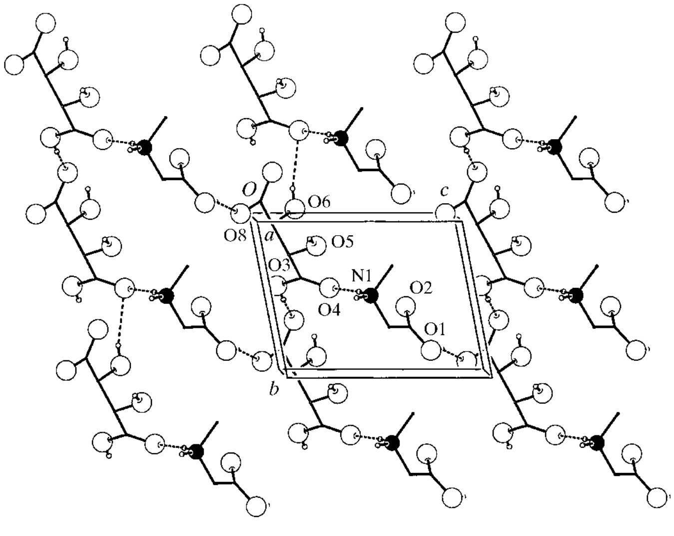


Figure 2
A view showing some of the O—H···O and N—H···O hydrogen bonds in (I).

Experimental

Colourless single crystals of the title complex were grown as transparent plates from a saturated aqueous solution containing sarcosine and tartaric acid in a 1:1 stoichiometric ratio.

Crystal data

$C_3H_8NO_2^+\cdot C_4H_5O_6^-$
$M_r = 239.18$
Triclinic, $P1$
$a = 5.0038\ (15)$ Å
$b = 6.442\ (2)$ Å
$c = 8.3179\ (11)$ Å
$\alpha = 78.60\ (2)^\circ$
$\beta = 80.62\ (2)^\circ$
$\gamma = 79.80\ (2)^\circ$
$V = 256.40\ (11)$ Å^3
$Z = 1$
$D_x = 1.549$ Mg m^{-3}
$D_m = 1.54$ Mg m^{-3}
D_m measured by flotation in carbon tetrachloride/xylene
Mo$K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 4$–17°
$\mu = 0.144$ mm^{-1}
$T = 293\ (2)$ K
Plate, colourless
$0.45 \times 0.30 \times 0.20$ mm

Data collection

Enraf–Nonius sealed-tube diffractometer
ω-2θ scans
1012 measured reflections
897 independent reflections
897 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\rm max} = 24.92^\circ$
$h = 0 \rightarrow 5$
$k = -7 \rightarrow 7$
$l = -9 \rightarrow 9$
2 standard reflections every 200 reflections intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.066$
$S = 1.089$
897 reflections
150 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.0215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.18$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}

All the H atoms were located from a difference Fourier map and then allowed for as riding atoms (C—H 0.96–0.98 Å, and N—H 0.90 and O—H 0.82 Å). The absolute configuration of this light-atom structure was not established by the analysis but is known from the configuration of the starting reagents.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$O8$^{\rm i}$	0.82	1.76	2.548 (2)	161
O3—H3$\cdots$O7$^{\rm ii}$	0.82	1.68	2.488 (2)	166
O5—H5$\cdots$O6$^{\rm iii}$	0.82	2.11	2.918 (2)	167
O6—H6$\cdots$O4$^{\rm iv}$	0.82	2.35	3.146 (2)	163
N1—H1$A\cdots$O4	0.90	2.05	2.946 (2)	174
N1—H1$B\cdots$O4$^{\rm iii}$	0.90	2.04	2.905 (2)	160
C2—H2$B\cdots$O2$^{\rm iii}$	0.97	2.23	3.074 (3)	145

Symmetry codes: (i) $x-1, 1+y, 1+z$; (ii) $x-1, 1+y, z$; (iii) $1+x, y, z$; (iv) $x, y-1, z$.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1993); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1116). Services for accessing these data are described at the back of the journal.

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