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Bis(DL-serinium) oxalate dihydrate

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In the title compound, $2C_3H_8NO_3^{+}\cdot.C_2O_4^{2-}\cdot 2H_2O$, the serine molecule exists in the cationic form with an uncharged carboxylic acid group and a positively charged amino group. The oxalic acid molecule exists as a double negatively charged oxalate anion. Two independent oxalate anions lie across inversion centres. The aggregation of individual molecules differs distinctly from other similar complexes.

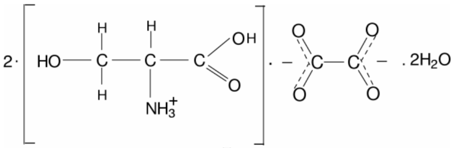
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.099
Data-to-parameter ratio = 11.3

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

Comment

Precise X-ray crystallographic investigations on complexes of amino acids with simple carboxylic acids, which are believed to have existed in the prebiotic earth (Miller & Orgel, 1974; Kvenvolden *et al.*, 1971), are expected to throw light on the nature of intermolecular interactions and biomolecular aggregation patterns (Vijayan, 1988; Prasad & Vijayan, 1993). Recently, a number of crystal structures of complexes of oxalic acid with glycine (Subha Nandhini *et al.*, 2001*a*), L-alanine (Subha Nandhini *et al.*, 2001*b*) and DL-alanine (Subha Nandhini *et al.*, 2001*c*), sarcosine (Krishnakumar *et al.*, 1999), DL-threonine (Subha Nandhini, Krishnakumar, Malathi *et al.*, 2001), L- and DL-histidine (Prabu *et al.*, 1996), L- and DL-arginine (Chandra *et al.*, 1998), and L- and DL-lysine (Venkatraman *et al.*, 1997) have been reported. The present study reports the crystal structure of the title compound, (I).



(I)

Serine exists in the cationic form with an uncharged carboxylic acid group and a positively charged amino group (Fig. 1). The oxalic acid molecule exists as a double negatively charged oxalate anion. Overall charge neutrality is achieved by a 2:1 stoichiometry, with the presence of two crystallographically independent serinium cations and a double negatively charged oxalate anion (uncommon in similar crystal structures) in the asymmetric unit. Two independent oxalate anions lie across inversion centres. In the crystal structure of the lysine–oxalic acid complex (Venkatraman *et al.*, 1997), the oxalic acid exhibits a double negatively charged ionization state. However, the situation is complex with the additional presence of two semi-oxalate anions.

The hydroxyl O atoms O3 and O3′ of the two independent serinium molecules participate both as acceptor and donor in hydrogen bonding (Table 1). Both the water molecules have a

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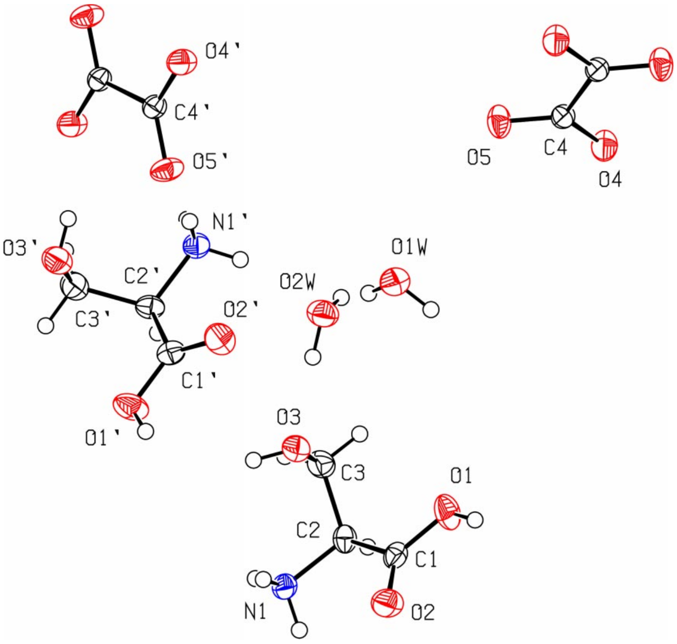

Figure 1
The molecular structure of (I) with atom-numbering scheme and 50% probability displacement ellipsoids.

similar tetrahedral hydrogen-bonding environment. There are no direct interactions between the amino acid molecules except for a C—H···O hydrogen bond connecting the molecules along the *a* axis (Fig. 2). The oxalate anions and water molecules mediate interactions between amino acid molecules in forming a three-dimensional network characterized by strong O—H···O and N—H···O hydrogen bonds. The aggregation of individual molecules differs distinctly from other similar complexes.

Experimental

Colorless single crystals of (I) were grown as transparent needles, from a saturated aqueous solution containing DL-serine and oxalic acid in a 1:1 stoichiometric ratio.

Crystal data

$2C_3H_8NO_3^+\cdot C_2O_4^{2-}\cdot 2H_2O$
$M_r = 336.26$
Monoclinic, $P2_1/c$
$a = 4.8685\ (10)$ Å
$b = 17.199\ (7)$ Å
$c = 17.172\ (4)$ Å
$\beta = 91.678\ (19)^\circ$
$V = 1437.2\ (7)$ Å^3
$Z = 4$
$D_x = 1.554$ Mg m^{-3}
$D_m = 1.56$ Mg m^{-3}
D_m measured by flotation in a mixture of xylene and bromoform
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 36$–45°
$\mu = 1.32$ mm^{-1}
$T = 293\ (2)$ K
Needle, colorless
$0.35 \times 0.20 \times 0.15$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
3513 measured reflections
2616 independent reflections
2528 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\rm max} = 67.9^\circ$
$h = -5 \rightarrow 0$
$k = 0 \rightarrow 20$
$l = -20 \rightarrow 20$
2 standard reflections every 200 reflections intensity decay: <1%

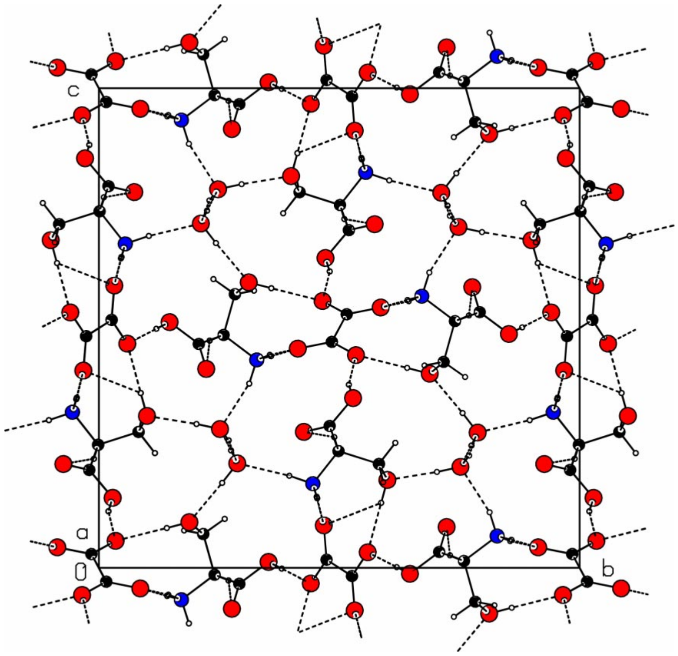

Figure 2
Packing diagram of (I) viewed down the *a* axis.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.099$
$S = 1.13$
2616 reflections
232 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.5233P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.25$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0521 (17)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1*W*	0.89	1.94	2.823 (2)	170
N1—H1*B*···O5^{i}	0.89	1.93	2.8129 (16)	174
N1—H1*C*···O5	0.89	2.06	2.9507 (18)	177
N1′—H1′1···O2*W*^{ii}	0.89	1.97	2.8254 (18)	160
N1′—H1′2···O5′^{iii}	0.89	1.91	2.8015 (16)	175
N1′—H1′3···O5′^{ii}	0.89	2.06	2.9431 (17)	174
O1′—H1′···O4^{i}	0.86 (3)	1.68 (3)	2.5374 (15)	174 (3)
O1—H1···O4′^{iv}	0.89 (3)	1.66 (3)	2.5158 (15)	160 (3)
O3—H3···O4^{v}	0.85 (3)	1.94 (3)	2.7696 (17)	166 (2)
O3′—H3′···O4′^{vi}	0.84 (3)	1.97 (3)	2.7718 (19)	161 (2)
O1*W*—H1*W*1···O3′	0.88 (3)	1.92 (3)	2.7778 (18)	163 (2)
O1*W*—H2*W*1···O2*W*	0.85 (3)	1.91 (3)	2.7552 (19)	170 (3)
O2*W*—H1*W*2···O1*W*^{iv}	0.84 (3)	2.01 (3)	2.8352 (18)	166 (3)
O2*W*—H2*W*2···O3^{vii}	0.88 (3)	1.86 (3)	2.7432 (19)	176 (2)
C2—H2···O2^{i}	0.98	2.38	3.2616 (19)	149
C2′—H2′···O2′^{iv}	0.98	2.32	3.2120 (19)	150

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

The H atoms were placed in calculated positions and were allowed to ride on their respective parent atoms using *SHELXL*97 (Sheldrick, 1997) defaults. H atoms bonded to O atoms were located from difference Fourier maps and were included in the refinement with isotropic displacement parameters. The O—H bond lengths are 0.84 (3)–0.89 (3) Å.

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*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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