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Glycinium oxalate

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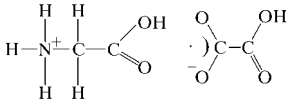
In the title compound, $C_2H_6NO_2^+\cdot C_2HO_4^-$, the glycine molecule exists in the cationic form and the oxalic acid molecule in the mono-ionized state. The molecules aggregate into alternate columns of glycinium and semi-oxalate ions. The structure is stabilized by an extensive network of hydrogen bonds.

Comment

Structural data on complexes of amino acids with carboxylic acids seem to be very limited. Single crystal X-ray investigations on such complexes are expected to throw light on the geometrical features of biomolecular interactions and aggregation patterns that might well have occurred in prebiotic polymerization (Vijayan, 1988; Prasad & Vijayan, 1993). The present study reports the crystal structure of a complex, (I), of glycine, the simplest of amino acids commonly found in proteins, with oxalic acid.



(I)

The glycine molecule exists in the cationic form with a positively charged amino group and an uncharged carboxylic acid group. The oxalic acid molecule exists in a mono-ionized state in the crystals. The crystal structure of the complex is illustrated in Fig. 2 and the hydrogen bonds that stabilize it are listed in Table 1. The glycine molecules form columns around 2_1 screw axes parallel to **b**. The molecules in each column are interconnected by a hydrogen bond between the amino and carboxyl groups of adjacent molecules, in a head-to-tail arrangement. Semi-oxalate ions also form columns parallel to **b**. Adjacent molecules are related by a cell translation and interconnected by an O—H···O hydrogen bond. Each such column and its equivalent generated by a centre of inversion connect two glycine columns giving rise to a double layer parallel to (102). In each layer, the unlike molecules are connected through an O—H···O hydrogen bond between the carboxyl group of the amino acid and the carboxylate group of the semi-oxalate ion, and their symmetry equivalents. The double layer is further stabilized by hydrogen bonds of the amino group of glycine with the semi-oxalate ion. The double layers are held together by possible C—H···O and van der Waals interactions. The mode of aggregation in the structure is different from those observed so far in amino acid–oxalic acid complexes (Bakke & Mostad, 1980; Prabu *et al.*, 1996; Chandra *et al.*, 1998; Krishnakumar *et al.*, 1999).

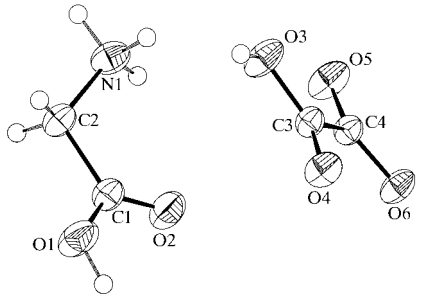


Figure 1
The molecular structure of (I) with the atom-numbering scheme and 50% probability displacement ellipsoids.

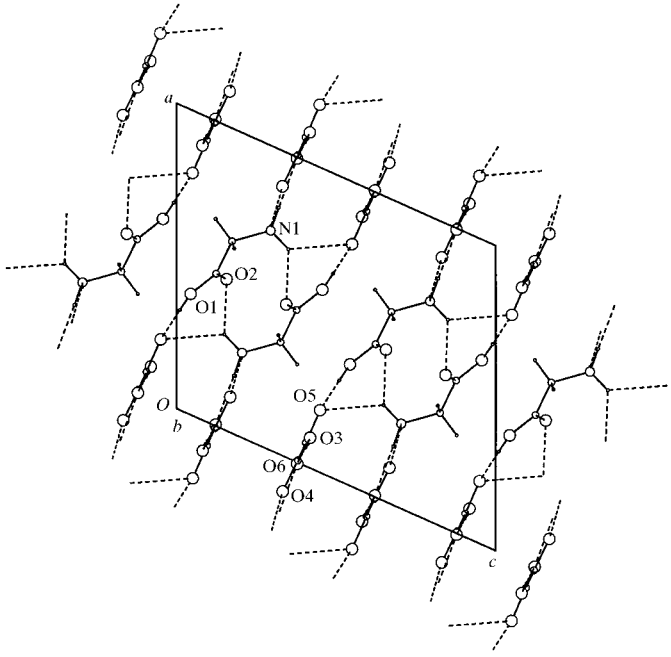


Figure 2
Packing diagram of the title molecule viewed down the *b* axis.

Experimental

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

Crystal data

$C_2H_6NO_2^+\cdot C_2HO_4^-$
M_r = 165.11
Monoclinic, $P2_1/c$
a = 10.5807 (15) Å
b = 5.650 (2) Å
c = 12.093 (3) Å
β = 113.830 (10)°
γ = 90.00 (2)°
V = 661.3 (3) Å^3
Z = 4
D_x = 1.658 Mg m^{-3}
D_m = 1.66 Mg m^{-3}

D_m measured by flotation in a mixture of carbon tetrachloride and xylene
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 16–29°
μ = 1.428 mm^{-1}
T = 293 (2) K
Plate, colourless
0.45 × 0.32 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.555, T_{max} = 0.730
1280 measured reflections
1212 independent reflections
1183 reflections with $I > 2\sigma(I)$

R_{int} = 0.013
θ_{max} = 70.03°
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 6$
$l = -14 \rightarrow 13$
2 standard reflections
every 200 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.106
S = 1.205
1212 reflections
129 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0580P)^2 + 0.2023P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.069 (4)

All the H atoms were located from a difference Fourier map and refined isotropically [C—H distances 0.90 (2) and 0.96 (2) 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, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O5^{i}	0.86 (3)	1.73 (3)	2.593 (2)	174 (3)
N1—H4···O4^{ii}	0.91 (3)	2.25 (3)	3.082 (2)	152 (2)
N1—H5···O2^{iii}	0.90 (3)	2.26 (3)	2.949 (2)	133 (2)
N1—H5···O5^{iv}	0.90 (3)	2.51 (2)	3.172 (2)	130 (2)
N1—H6···O6^{v}	0.94 (2)	1.81 (2)	2.698 (2)	156 (2)
O3—H7···O6^{vi}	0.89 (3)	1.65 (3)	2.540 (2)	177 (2)
C2—H2···O5	0.96 (2)	2.53 (2)	3.314 (2)	139 (2)

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1115). Services for accessing these data are described at the back of the journal.

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