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Glycinium maleate

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In the title compound, $C_2H_6NO_2^+\cdot C_4H_3O_4^-$, the glycine molecule exists in the cationic form with a positively charged amino group and an uncharged carboxylic acid group. The maleic acid molecule exists in a mono-ionized state. In the semimaleate ion, an intramolecular OH···O hydrogen bond is found to be asymmetric. The glycinium and semimaleate ions aggregate into alternate columns extending along the *c* axis. A C—H···O hydrogen bond is also observed.

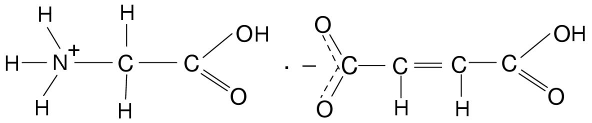
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.082
Data-to-parameter ratio = 9.6

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

Comment

Glycine remains one of the most extensively studied amino acids as it is known to form innumerable complexes with metals, inorganic salts and inorganic acids. However, structural data on complexes of organic acids with amino acids in general, particularly glycine, seem to be very limited. A series of investigations is being carried out in our laboratory to obtain structural information on biomolecular interactions and characteristic aggregation patterns of amino acid–carboxylic acid complexes, at atomic resolution. The present study reports the crystal structure of (I), a complex of glycine with maleic acid. Recently, the crystal structure of a complex of glycine with oxalic acid (Subha Nandhini *et al.*, 2001) has been reported.



(I)

Fig. 1 shows the molecular strcuture with the atom-numbering scheme. The glycine molecule exists in the cationic form with a positively charged amino group and an uncharged carboxylic acid group. The maleic acid molecule exists in a mono-ionized state. The semimaleate ion is essentially planar as observed in the crystal structures of similar complexes. In the semimaleate ion, an intramolecular hydrogen bond between atoms O3 and O5 is found to be asymmetric, as in the crystal structure of maleic acid (James & Williams, 1974). However, in the crystal structures of complexes of maleic acid with DL- and L- arginine (Ravishankar *et al.*, 1998), and L-histidine and L-lysine (Pratap *et al.*, 2000), this intramolecular hydrogen bond between the carboxylic acid and carboxylate groups is symmetric with a H atom shared between the respective O atoms.

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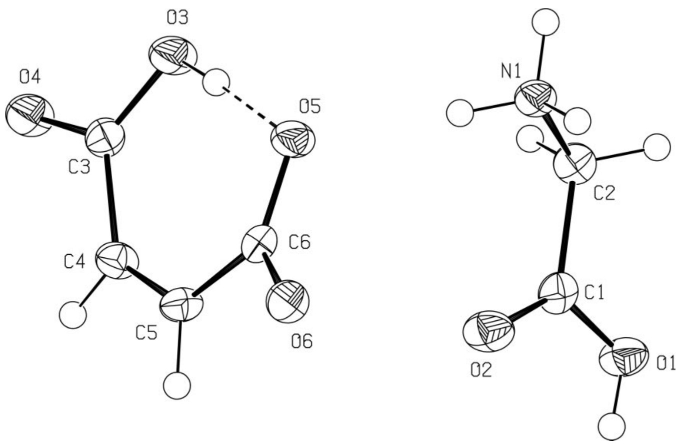

Figure 1
The molecular structure of (I) with the atom-numbering scheme and 50% probability displacement ellipsoids.

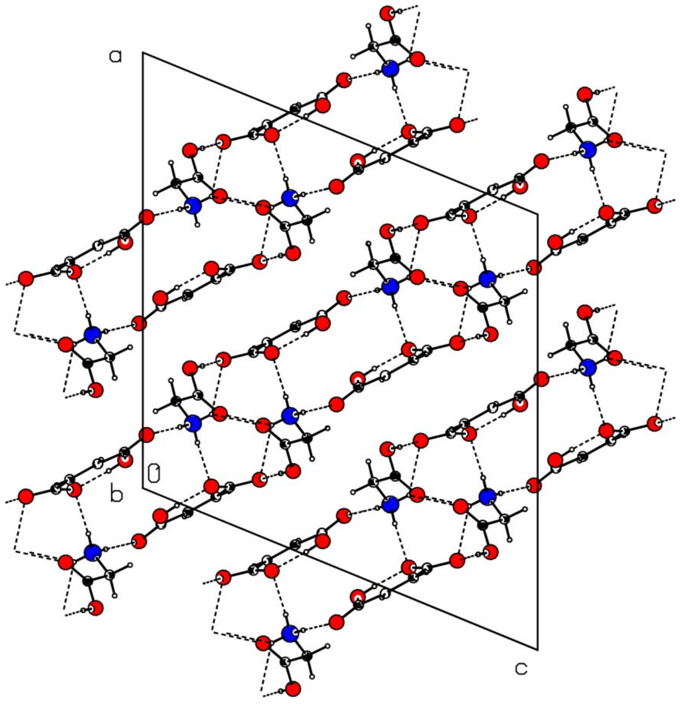

Figure 2
Packing of the molecules of (I) viewed down the *b* axis.

The packing of molecules of (I) within the unit cell viewed down the *b* axis is shown in Fig. 2. The glycinium and semimaleate ions aggregate into alternate columns extending along the *c* axis. In these columns, the molecules related by a centre of inversion form hydrogen-bonded double layers parallel to the diagonal of the *ac* plane. No hydrogen bond is observed between these double layers, which they are held together by van der Waals interactions. A head-to-tail hydrogen bond between the glide-related glycinium ions is present. The mode of aggregation of molecules in the crystal structure is similar to that observed in glycinium oxalate (Subha Nandhini *et al.*, 2001).

Experimental

Colorless prismatic single crystals of (I) were grown from a saturated aqueous solution containing glycine and maleic acid in a stoichiometric ratio of 1:1.

Crystal data

$C_2H_6NO_2^+ \cdot C_4H_3O_4^-$
$M_r = 191.14$
Monoclinic, $C2/c$
$a = 17.689$ (4) Å
$b = 5.6610$ (11) Å
$c = 17.328$ (4) Å
$\beta = 112.30$ (3)°
$V = 1605.4$ (6) Å^3
$Z = 8$
$D_x = 1.582$ Mg m^{-3}
$D_m = 1.58$ (3) Mg m^{-3}
D_m measured by flotation in a mixture of bromoform and xylene
Mo $K\alpha$ radiation
Cell parameters from 1024 reflections
$\theta = 2.5$–23.0°
$\mu = 0.14$ mm^{-1}
$T = 293$ (2) K
Prismatic, colourless
0.5 × 0.3 × 0.3 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multiscan (*SADABS*; Bruker, 1998)
$T_{\min} = 0.933$, $T_{\max} = 0.959$
6136 measured reflections
1161 independent reflections
1091 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 23.3°$
$h = -19 \rightarrow 19$
$k = -6 \rightarrow 6$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.082$
$S = 1.11$
1161 reflections
121 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 1.7034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0020 (6)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1\cdots O6^{i}$	0.82	1.77	2.5861 (17)	171
$O3-H3\cdots O5$	0.82	1.63	2.4465 (19)	176
$N1-H1A\cdots O4^{ii}$	0.89	1.92	2.8051 (18)	171
$N1-H1B\cdots O5^{iii}$	0.89	2.01	2.8960 (19)	173
$N1-H1C\cdots O2^{iv}$	0.89	2.15	2.8791 (19)	139
$N1-H1C\cdots O6^{v}$	0.89	2.30	2.951 (2)	130
$C2-H2A\cdots O1^{vi}$	0.97	2.58	3.320 (2)	133

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

H-atom positions were generated geometrically and the H atoms were allowed to ride on their respective parent atoms with *SHELXL*97 (Sheldrick, 1997) defaults for bond lengths. The torsion angles about the C—O bonds of the hydroxyl groups were allowed to refine.

Data collection: *SMART–NT* (Bruker, 1999); cell refinement: *SMART–NT*; data reduction: *SAINT–NT* (Bruker, 1999); 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.

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