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Glycinium 3-nitrophthalate

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Key indicators

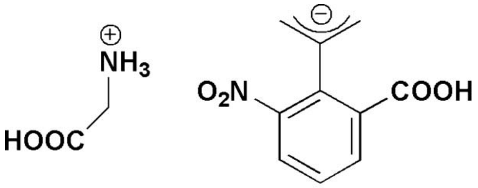
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.131
Data-to-parameter ratio = 9.3

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

In the title compound, $C_2H_6NO_2^+\cdot C_8H_4NO_6^-$, the cations and anions are self-assembled into chains by N—H···O and O—H···O hydrogen bonds, respectively. The two chains are held together by further N—H···O hydrogen bonds, resulting in a two-dimensional sheet.

Comment

There is increasing interest in the structures of the salts of organic acids with amino acids such as glycine (Rajagopal *et al.*, 2001). We describe here the synthesis and crystal structure of the title compound, (I), which is a molecular salt of glycine and 3-nitrophthalic acid (Fig. 1).



(I)

In the structure of (I), glycine and 3-nitrophthalic acid form a salt, with the H atom transferred from the carboxyl group adjacent to the nitro substituent of 3-nitrophthalic acid to the amine group of glycine. The C10—O5 and C10—O6 bond lengths of 1.279 (2) and 1.225 (2) Å, respectively, imply some delocalization of the charge of this carboxylate group. The C9—O3 and C9—O4 bond lengths are 1.321 (2) and 1.206 (2) Å, respectively, suggesting that the H atom is bonded to atom O3, which is consistent with the location of H in a difference Fourier map. The plane of the nitro group makes a

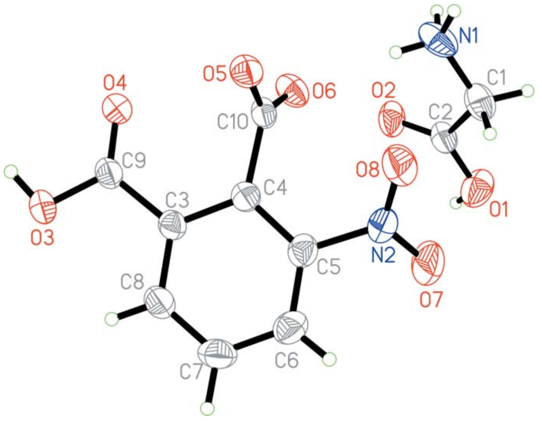


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

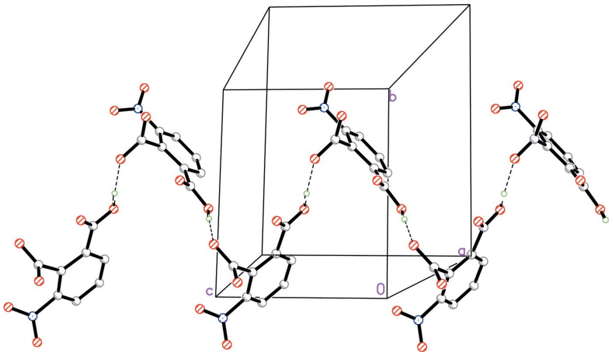


Figure 2
Part of the crystal structure of (I), showing the chain structure of 3-nitrophthalate anions linked by hydrogen bonds (dashed lines).

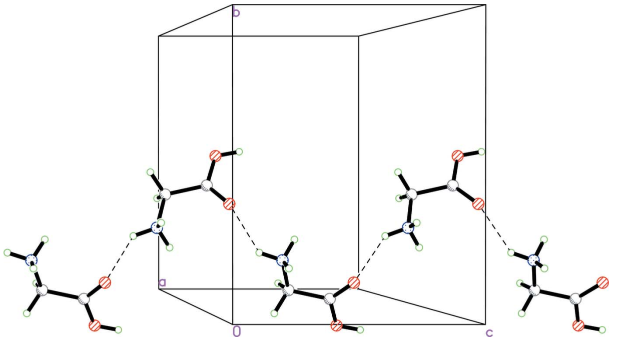


Figure 3
Part of the crystal structure of (I), showing the chain structure of glycinium cations linked by hydrogen bonds (dashed lines).

dihedral angle of 35.7 (3)° with the mean plane of the benzene ring. The delocalized carboxylate group is close to perpendicular to the benzene ring, with a dihedral angle of 74.80 (12)°, while the unionized carboxylic acid group is approximately coplanar with the ring [dihedral angle 11.3 (3)°]. The orthogonal arrangement of the carboxylate group lying between the nitro and the unionized carboxylic acid group may occur to reduce steric hindrance.

The C2—O1 and C2—O2 bond lengths of the glycinium cation are 1.311 (3) and 1.197 (3) Å, respectively, suggesting that the H atom is bonded to atom O1, which is also consistent with the location of H in a difference map.

In the crystal structure of (I), carboxyl atom O3 acts as hydrogen-bond donor to delocalized carboxylate atom O5 of an adjacent 3-nitrophthalate anion, producing a chain structure of the anions running along the [001] direction (Fig. 2), similar to that found in 3-nitrophthalic acid co-crystal complexes (Glidewell *et al.*, 2003, 2005). Ammonium atom N1 of the cation acts as a hydrogen-bond donor to neighbouring glycinium carboxyl atom O2, also leading to a chain structure of cations running along [001] (Fig. 3). These cationic chains lie in between the anionic chains and link them into a two-dimensional sheet through further N—H···O hydrogen bonds (Fig. 4). Inter-layer interactions are dominated by van der Waals forces.

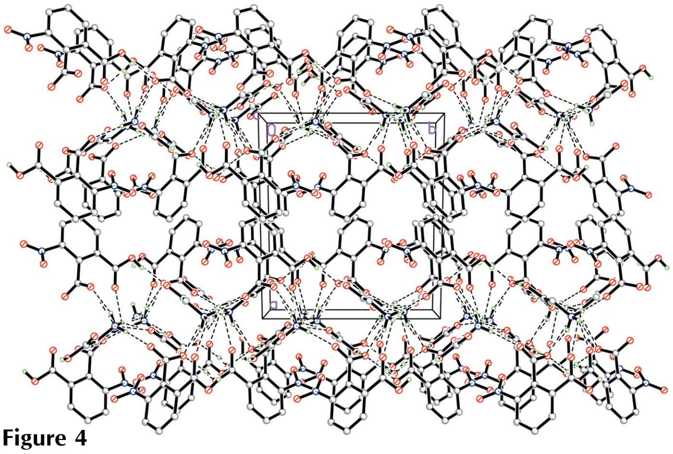


Figure 4
A packing diagram for (I), showing the two-dimensional sheet structure. Dashed lines indicate hydrogen bonds.

Experimental

Equimolar quantities (1 mmol) of glycine and 3-nitrophthalic acid in water (10 ml) were mixed and heated to 378 K. Upon evaporation, crystals of (I) suitable for single-crystal X-ray diffraction were obtained.

Crystal data

$C_2H_6NO_2^+ \cdot C_8H_4NO_6^-$
M_r = 286.20
Monoclinic, $P2_1/c$
a = 12.965 (3) Å
b = 10.966 (2) Å
c = 8.6833 (17) Å
β = 107.61 (3)°
V = 1176.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 298 (2) K
0.25 × 0.18 × 0.12 mm

Data collection

Siemens SMART CCD 1000 area-detector diffractometer
Absorption correction: none
2221 measured reflections
2072 independent reflections
1735 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.131
S = 1.05
2072 reflections
222 parameters
5 restraints
All H-atom parameters refined
$\Delta\rho_{\rm max}$ = 0.44 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H2···O6	0.864 (18)	2.116 (18)	2.979 (3)	176 (3)
N1—H3···O5$^{\rm i}$	0.862 (18)	2.02 (2)	2.845 (3)	160 (3)
N1—H1···O2$^{\rm ii}$	0.853 (19)	2.05 (3)	2.717 (2)	135 (3)
O1—H4···O5$^{\rm iii}$	0.863 (19)	1.86 (2)	2.725 (2)	178 (4)
O3—H5···O5$^{\rm iv}$	0.858 (18)	1.722 (19)	2.571 (2)	170 (3)

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

All H atoms were located in a difference map and their positions and $U_{\rm iso}$ values were freely refined. Refined C— distances are in the range 0.88 (3)–0.97 (3) Å.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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