

## Glycine sodium nitrate

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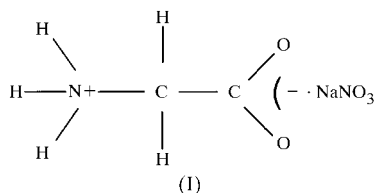
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The glycine molecule in the title compound, Na(NO<sub>3</sub>)·C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>, exists in the zwitterionic form. The Na atom exhibits eightfold coordination and the polyhedron may be visualized as a distorted hexagonal bipyramid. The glycine molecules are linked through head-to-tail hydrogen bonds and are found 'sandwiched' between the Na(NO<sub>3</sub>) layers.

## Comment

Glycine has the distinction of being the only amino acid which forms many addition compounds with inorganic acids and salts, besides forming metallic complexes. The present study of the title compound, (I), seems to be the only work on an amino acid complex which contains both sodium and nitrate ions. The crystal structures of glycine sodium iodide hydrate (Verbist *et al.*, 1971) and glycine potassium triiodide (Herbststein & Kapon, 1980) are the only other complexes involving glycine and alkali metals that have been reported so far.



The glycine molecule in (I) exists in the zwitterionic form. The nitrate group exhibits non-crystallographic  $D_{3h}$  symmetry, with the three N—O bond distances having equal values [mean 1.241 (5) Å] and the three O—N—O angles not deviating significantly from 120°. Fig. 1 shows the coordination environment around the Na atom, which has a coordination number of eight. The coordination polyhedron may be visualized as a distorted hexagonal bipyramid, with the carboxyl O atoms of the amino acid group occupying the apical sites. The Na—O distances range from 2.324 (3) to 2.719 (3) Å.

Fig. 2 shows the layer formed by the sodium and nitrate ions, in which the O atoms of the nitrate groups coordinate to Na, forming a two-dimensional layered network. These layers are separated by a distance of  $a/2$  and are interconnected

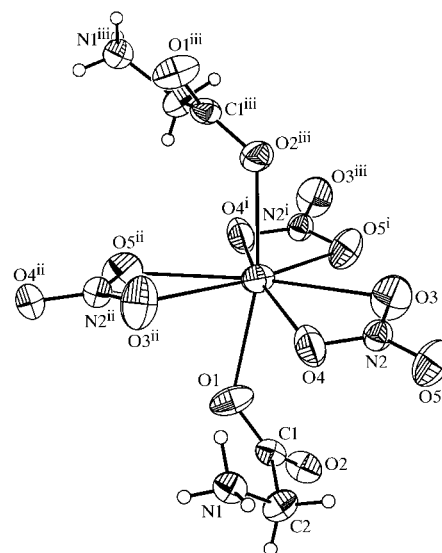


Figure 1

The molecular structure of (I) showing the coordination environment around Na. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii [symmetry codes: (i)  $x, 1 - y, z$ ; (ii)  $x, 1 - y, z - \frac{1}{2}$ ; (iii)  $x - \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$ ].

through coordination of the carboxyl O atoms of the glycine molecules to Na. Almost linear O1—Na—O2 chains involving carboxyl O atoms run along the  $(20\bar{2})$  plane in the  $[101]$  direction.

The glycine molecules are seen 'sandwiched' between layers of Na(NO<sub>3</sub>) (Fig. 3). Both carboxyl O atoms participate in hydrogen bonding as acceptors, forming two N—H···O head-to-tail hydrogen bonds, one along the  $b$  direction and the other related to it by a  $c$  glide. In addition, an N—H···O and a

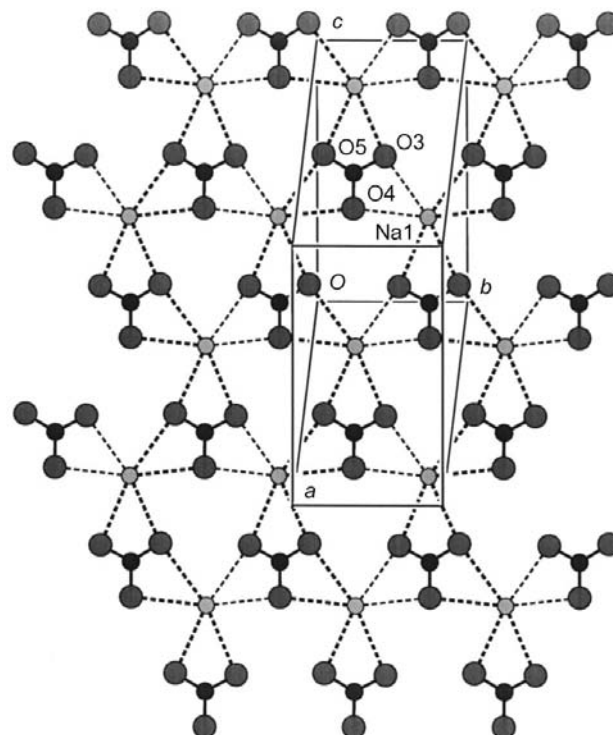
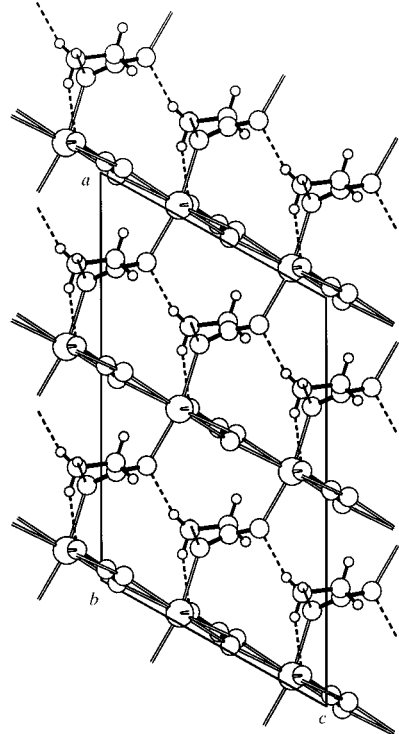


Figure 2

A view showing the O atoms of the nitrate groups coordinating to Na atoms, forming a two-dimensional layered network.

C—H...O hydrogen bond are also observed, involving atom O4 of the nitrate group as acceptor.



**Figure 3**  
The unit-cell packing of molecules of (I), showing the glycine molecules 'sandwiched' between the Na(NO<sub>3</sub>) layers.

Interestingly, in the crystal structure of glycine silver nitrate (Mohana Rao & Viswamitra, 1972), which is found to be ferroelectric below 218 K (Pepinsky *et al.*, 1957), all three H atoms attached to the N atom are shared by the O atoms of the nitrate group in forming hydrogen bonds, and the carboxyl O atoms of the amino acid molecule do not take part in the hydrogen-bonding network.

## Experimental

Colourless single crystals of (I) were grown as transparent plates from a saturated aqueous solution containing glycine and sodium nitrate in a stoichiometric ratio.

### Crystal data

Na(NO<sub>3</sub>)·C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>  
*M<sub>r</sub>* = 160.07  
 Monoclinic, *Cc*  
*a* = 14.329 (3) Å  
*b* = 5.2662 (11) Å  
*c* = 9.1129 (18) Å  
 $\beta$  = 119.10 (3)°  
*V* = 600.9 (2) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.769 Mg m<sup>-3</sup>  
*D<sub>m</sub>* = 1.76 Mg m<sup>-3</sup>

*D<sub>m</sub>* measured by flotation in a mixture of carbon tetrachloride and bromoform  
 Mo *K*α radiation  
 Cell parameters from 25 reflections  
 $\theta$  = 7–16°  
 $\mu$  = 0.23 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Plate, colourless  
 0.32 × 0.21 × 0.18 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer  
 $\omega/2\theta$  scans  
 1077 measured reflections  
 531 independent reflections  
 523 reflections with  $I > 2\sigma(I)$   
*R<sub>int</sub>* = 0.017

$\theta_{\max}$  = 25°  
*h* = -16 → 5  
*k* = -5 → 6  
*l* = -9 → 10  
 2 standard reflections  
 frequency: 60 min  
 intensity decay: <2%

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.029  
*wR*(*F*<sup>2</sup>) = 0.078  
*S* = 1.07  
 531 reflections  
 92 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.1988P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.26 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.28 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.020 (4)

**Table 1**

Selected bond lengths (Å).

Na1—O1	2.410 (3)	Na1—O4	2.647 (3)
Na1—O2 <sup>i</sup>	2.324 (3)	Na1—O4 <sup>iii</sup>	2.669 (3)
Na1—O3	2.615 (3)	Na1—O5 <sup>iii</sup>	2.719 (3)
Na1—O3 <sup>ii</sup>	2.655 (3)	Na1—O5 <sup>ii</sup>	2.615 (3)

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

**Table 2**

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1A...O1 <sup>i</sup>	0.89	2.03	2.789 (4)	142
N1—H1B...O2 <sup>ii</sup>	0.89	1.97	2.780 (3)	151
C2—H2A...O4 <sup>iii</sup>	0.97	2.54	3.256 (4)	131
N1—H1C...O4	0.89	2.06	2.893 (4)	155

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

All H atoms were located from a difference Fourier map and were allowed to ride on their parent atoms, with default values for bond distances (as given in Table 2) and displacement parameters. Friedel pairs were merged before the final refinement cycles.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS93* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1628). Services for accessing these data are described at the back of the journal.

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