

Table 1. *X-ray pattern for NaLiSO₄ at 556° C.*

Cu K α radiation		
2θ (°)	$1/d^2$ (Å ⁻²)	Relative intensities
21.75	0.0601	10
31.0	0.1202	2
38.2	0.1804	1

These lines may be indexed by means of a cubic body-centered unit cell with an edge length of 5.77 Å. A density of 2.18 g.cm.⁻³ is calculated with two formula units of NaLiSO₄ in the cell. (By indexing the pattern as primitive cubic, the density would have been 3.08 g.cm.⁻³ with two formula units in the cell, or 1.54 g.cm.⁻³ with one formula unit in the cell. The former density is too high, and the latter too low.)

Space-group considerations are probably of limited value in determining the atomic positions in NaLiSO₄. Coupled rotation of the sulfate groups, together with translations of the cations, are likely to occur, as in cubic

lithium sulfate. The electrical conductivities of LiNaSO₄, as that of Li₂SO₄, were found to be of the same magnitude in the high-temperature modification and in the fused state (Förland & Krogh-Moe, unpublished). Thus it is not possible to assign definite single positions to the oxygens or the cations in the lattice. The sulfur remain fixed in the (0, 0, 0) and ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) positions.

The average volume per sulfate ion increases about 10% on adding 30 mole% sodium sulfate to cubic lithium sulfate. The sulfate ion volume is nearly the same with a sodium sulfate content of 30 mole% as with a content of 50 mole%. This demonstrates that the structural change from face centered to body centered results in a more efficient packing of the anions and the cations.

References

- FÖRLAND, T. & KROGH-MOE, J. (1957). *Acta Chem. Scand.* **11**, 565.
 NACKEN, R. (1907). *N. Jb. Min. Geol. A*, **24**, 1.

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The crystal structure of γ -glycine. By YOICHI IITAKA, *Mineralogical Institute, Science Department, University of Tokyo, Hongo, Tokyo, Japan*

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In a previous paper, the author reported on a new form of glycine. This new form, designated as γ -glycine, is strongly piezoelectric, and crystallizes with trigonal hemihedral symmetry. The space group is either $P3_1$ or $P3_2$, and the unit cell contains three molecules (Iitaka, 1954). The redetermination of the unit-cell dimensions gave

$$a = 7.037, \quad c = 5.483 \text{ \AA}.$$

In the following, a brief account of the structure determination of γ -glycine will be given. We shall describe the structure, comparing it with that of α -glycine (Albrecht & Corey, 1939; Marsh, 1957). Intensity data obtained from both oscillation and Weissenberg photographs were used.

The crystal shows a marked piezoelectric property along the c axis. The length of this axis is nearly equal to the c axis of α -glycine, the latter corresponding to the intermolecular distance arranged head-to-tail. These facts suggest that the dipolar molecules are arranged along the c axis. From the Harker section at $z = \frac{1}{3}$, it was possible to obtain approximate parameter values, x and y , for the oxygen, nitrogen and carbon atoms. Using conventional bond distances and bond angles for the molecule, and the hydrogen bond distance $\text{NH} \cdots \text{O}$ for nitrogen and oxygen atoms in neighbouring molecules, a satisfactory atomic arrangement was derived.

The refinement of the structure was carried out, using both ($hk0$) and ($0kl$) Fourier and difference Fourier projections, followed by three-dimensional structure-factor calculations. No further shifts of significance were indicated in the sixth ($0kl$) projection. At the present stage, the reliability indices are 0.14, 0.12 and 0.15 for ($0kl$), ($hk0$) and (hkl) reflexions, respectively, neglecting con-

tributions from hydrogen atoms. The Fourier projection along the a axis is shown in Fig. 1.

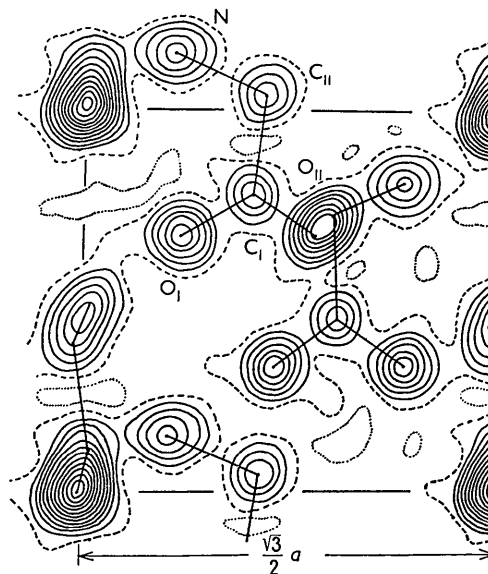


Fig. 1. The a -axis Fourier projection for γ -glycine. Contours at intervals of 2 e. \AA^{-2} . Dotted lines indicate 0 e. \AA^{-2} , and broken lines 2 e. \AA^{-2} .

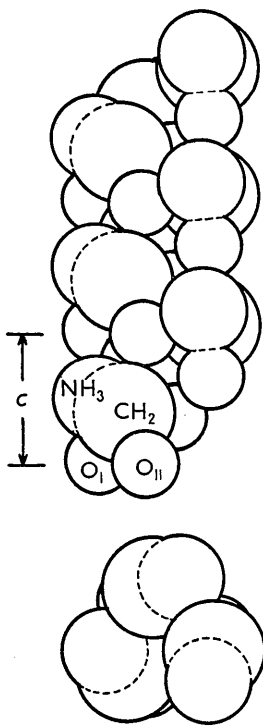
The shape of the molecule is found to be nearly the same as that of α -glycine. In Table 1, the bond distances and bond angles are given, together with the values

Table 1. Bond distances and bond angles in γ - and α -glycine

	γ -Glycine	α -Glycine*		γ -Glycine	α -Glycine*
N-C _{II}	1.46 Å	1.474 Å	C _I -C _{II} -N	107°	111.8°
C _I -C _{II}	1.53	1.523	O _I -C _I -C _{II}	122	117.4
C _I -O _I	1.29	1.252	O _{II} -C _I -C _{II}	114	117.1
C _I -O _{II}	1.22	1.255	O _I -C _I -O _{II}	122	125.5
		± 0.005			± 0.3

* Corey, 1957; Marsh, 1957.

recently redetermined in α -glycine (Marsh, 1957). The nitrogen atom of the molecule lies, as in α -glycine, a short distance out of the plane containing the carboxyl group and the α -carbon atom. This twist about the C-N bond makes the molecule asymmetric. These molecules are arranged in a helical chain, each pitch containing three molecules. These chains are packed in parallel along the c axis. A single chain is shown in Fig. 2.

Fig. 2. The chain of glycine molecules found in γ -glycine.

Each nitrogen atom is surrounded by five immediate oxygen neighbours at short distances (Table 2). In fact, three of them, O_I^C, O_{II}^A and O_I^{A'} are arranged approx-

imately in tetrahedral directions with respect to the N-C bond, and they are so close to the nitrogen atom that it is suggested they take part in hydrogen bonds. From the N...O distances, it appears that two hydrogen atoms attached to a nitrogen atom strongly link this nitrogen atom with two oxygen atoms of adjacent molecules in the same chain, while there is still one more hydrogen atom linking the same nitrogen atom with an oxygen atom of the adjacent chain. The molecule seems to be taken as a zwitter-ion.

The juxtaposition of parallel chains is such that dipolar interactions between molecules stabilize the molecular arrangement. Each nitrogen atom is surrounded by oxygen atoms, and each oxygen atom by nitrogen atoms, so that electrostatic interactions, if any exist, also favour the structure.

It is interesting to see that in γ -glycine one and the same kind of asymmetric molecules crystallize into one of the enantiomorphous forms, whereas in α -glycine two enantiomorphous molecules are related by a centre of symmetry, as in the case of racemic acids. Further, in spite of the entirely different molecular arrangements, the role of hydrogen bonds and other interactions arising from the structure seems somewhat similar in the two forms of glycine. Full details will be published soon.

I have examined β -glycine and find that the β form exhibits a definite piezoelectric property. Further study of this substance is now in progress.

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References

- ALBRECHT, G. & COREY, R. B. (1939). *J. Amer. Chem. Soc.* **61**, 1087.
 COREY, R. (1957). Private communication.
 IITAKA, Y. (1954). *Proc. Japan Acad.* **30**, 109.
 MARSH, R. E. (1957). Fourth International Congress of Crystallography, Paper No. 8.1 (*Acta Cryst.* (1957), **10**, 814).

Table 2. N...O interatomic distances, and C-N...O angles

	N...O _I ^C	N...O _{II} ^A	N...O _I ^{A'}	N...O _I ^{B'}	N...O _{II} ^B
N...O (Å)	2.80	2.81	2.95	2.89	3.01
C-N...O (°)	111	91	124	161	89