

The conclusion to be drawn from these calculations is that the zigzag model of the molecule fits the *experimental atomic coordinates* better than the planar model given by Iball & Young, and that there is less than one chance in forty that this improvement in fit is fortuitous. More accurate experimental results are needed before a decision can be made between the simple zigzag model discussed above or a more complex one. It is also not clear at present whether the deviation from a planar shape is a property of the free molecule or whether this should be ascribed to packing effects. Results from a three-dimensional analysis now in progress (Iball, 1960) should help to settle these points.

The method used for fitting planes to various sets of atomic coordinates by least squares was that given by Schomaker, Waser, Bergmann & Marsh (1959). Its use in the present problem has been facilitated by a pro-

gramme prepared for the Stantec Zebra electronic computer in our laboratory by Mr G. J. Rudolph, whose assistance is greatly appreciated. I am also indebted to Prof. A. J. B. Wiid, Mr C. R. Troskie and Mr G. Gafner for helpful discussions and to Dr J. N. van Niekerk for his interest in this work.

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Comments on the properties of triglycine sulfate. By A. D. BALLATO, *U.S. Army Signal Research and Development Laboratory, Fort Monmouth, New Jersey, U.S.A.*

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A recent paper by Konstantinova, Sil'vestrona & Aleksandrov (1959) has described the preparation and measurement of triglycine sulfate, where the piezoelectric strain constants $d_{i\mu}$ were obtained by the resonance-anti-resonance method using ϵ^S , the clamped dielectric constant.

Bechmann (1954) has shown that in this case the $d_{i\mu}$ must be computed using ϵ^m , the effective dielectric constant for the mode considered. Since only in the measurement of d_{16} , d_{34} , and d_{22} where thickness shear vibrations are used, can the effective dielectric constant be considered that at constant strain, the determination of the remaining $d_{i\mu}$ must be considered subject to a greater factor of uncertainty than the authors give.

This uncertainty is not so great for d_{14} and d_{36} as it is for d_{21} , d_{23} , and d_{25} since contour modes were used for the former and longitudinal vibrations for the latter. The magnitude of error cannot be calculated because of the paucity of data given, but an estimate may be made using the curves showing the vibration of the dielectric constant ϵ_{22} as a function of frequency for various values of field strength. The curve corresponding to lowest field strength shows a variation of greater than ten to one over the range of frequencies which correspond to the dielectric constants ϵ^T and ϵ^S . The effective piezoelectric constant ρ is proportional to $1/\epsilon$, and so could vary by more than three to one; however, since ϵ^m is between ϵ^T and ϵ^S , this figure gives only an upper bound. The actual error is probably small for all constants with the exceptions noted above.

It should also be pointed out that some of the values for the compliances s^D calculated from the stiffnesses measured by the ultrasonic method are incorrect. The proper values are given below; the calculations were

carried out on the Burroughs Datatron 220 computer in use at this Laboratory, using a matrix inverting program based on the Crout procedure (Hildebrand, 1952).

Table 1. *Elastic compliances s_{ik} for triglycine sulfate*
 Computed from data of

V. P. Konstantinova, I. M. Sil'vestrona & K. S. Aleksandrov.

| Elastic compliances | Values |
|---------------------|-----------------------------------|
| | 10^{-13} cm. ² /dyne |
| s_{1k} | |
| s_{11} | 32.9 |
| s_{22} | 69.8 |
| s_{33} | 108.5 |
| s_{44} | 105.4 |
| s_{55} | 107.3 |
| s_{66} | 161.5 |
| s_{23} | -57.7 |
| s_{13} | -22.7 |
| s_{12} | -2.9 |
| s_{15} | -1.4 |
| s_{25} | -24.5 |
| s_{35} | 40.9 |
| s_{46} | 4.4 |

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