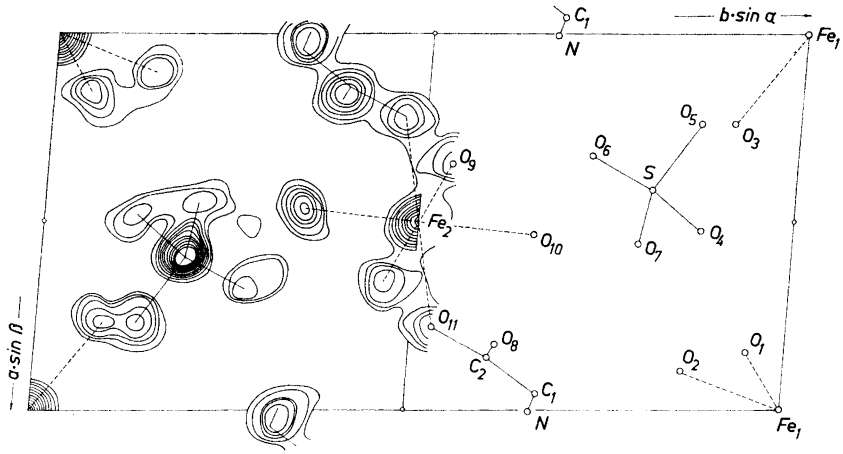

Fig. 1b Iron (II) sulfate pentahydrate glycine: *c* axis projection, showing the complete unit cell. Electron density contours are drawn for the unique portion to the left and the corresponding atomic positions are indicated to the right across the center of symmetry.

Average temperature factors for the two projections, (B *hk*0) : oxygen 3.0, carbon 3.8, nitrogen 3.4, sulfur 1.51, iron 1.62 Å², B (0*kl*): oxygen 2.5, carbon 3.3, nitrogen 2.9, sulfur 0.89, iron 1.00 Å². The residual error indices are R (*kh*0) = 0.14, R (0*kl*) = 0.18.

The structure is shown together with two electron density maps in Fig. 1*a* and *b*. It is built up of two different kinds of complex cations: $Fe(H_2O)_6^{2+}$ and $Fe(H_2O)_4(^-OOCCH_2NH_3^+)_2^{2+}$. In the latter ion one of the oxygen atoms of the carboxyl group in the glycine »Zwitterion» is bonded to the central Fe^{2+} ion. The two glycine molecules are in trans positions. These complex cations obviously can build up a structure, together with the sulphate ions, with more favorable lattice energy than one containing only one type of cation $Fe(H_2O)_5(^-OOCCH_2NH_3^+)^{2+}$. The accuracy of the structure determination does not permit a detailed discussion of the bond lengths but it is quite clear that a complicated hydrogen bridge system joins the different parts of the structure. The aim with this structure determination has, however, only been to establish the co-ordination around the Fe^{2+} ions and this problem has been definitely solved. Every suggestion about chelate bonding with the amino group can thus be rejected.

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A Note on the Structure of Barium Tetraborate

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Crystalline barium tetraborate, $BaO \cdot 4B_2O_3$, was obtained by Levin and McMurdie as a congruently melting phase in the system barium oxide — boron oxide[1]. Single crystals of this phase were prepared during the present study by fusing barium carbonate with the calculated amount of boric acid in a platinum

crucible at 1 000°C, and crystallizing the melt at 800°C. Weissenberg and oscillation X-ray photographs, taken about three axes of these crystals, showed an orthorhombic symmetry with the following unit cell dimensions:

$$a = 8.56 \text{ Å}$$
$$b = 2 \times 8.69 \text{ Å}$$
$$c = 13.20 \text{ Å}$$

A very weak doubling along the b axes was observed and is indicated in the above figures by writing 2×8.69 Å instead of 17.38 Å. The calculated density is 2.91 g/cm³ with 8 formula units of $BaO \cdot 4B_2O_3$ in the cell.

The Weissenberg diagrams disclose a pronounced pseudo tetragonal symmetry of barium tetraborate. This agrees with the optical properties of the compound. Thus Levin and McMurdie were unable to decide whether the crystals were uniaxial or biaxial negative [1]. The same authors also noted that the crystals exhibit polysynthetic twinning. Some of the present X-ray diagrams show twinning, in which the twins have paralell c-axes with the 010 plane facing the 100 plane.

Approximate barium positions can be determined by inspecting the X-ray diagrams. From the rotation diagram around the c-axes it is seen that the general hkl reflections are on average considerably stronger for even values of l than for odd. Therefore, as a first approximation, a reduced cell with halved b and c axes may be considered for the heavy barium atoms. This pseudo cell contains two barium atoms. Further information is obtained from equatorial and non-equatorial Weissenberg photograms. It is found that reflections are often weak or missing whenever $h + k' + l' = 2n + 1$. Here the indices k' and l' ($= l/2$) refer to the pseudo cell with halved b and c axes. This partially fulfilled condition of systematic extinctions suggests an approximately body-centered arrangement of the barium atoms in the pseudo cell, where the barium atoms thus can be given the preliminary parameter values 0,0,0 and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$. The shortest distance between two barium atoms is 6.94 Å with these parameter values.

The correct space group of barium tetraborate is difficult to decide because of the pseudo symmetries. The final space group determination will therefore have to await further work.

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