The Structure of Barium Tetrathionate

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The crystals of the salt, $BaS_4O_6 \cdot 2H_2O$, are monoclinic prismatic [1]; $a = 5.17$ Å, $b = 9.46$ Å, $c = 19.07$ Å, $\beta = 96°$. There are four molecules per unit cell; space group, $C_{2h}^5 - P2_1/c$. The present note gives preliminary results of a crystal structure analysis of the dihydrate.

Intensities of the reflections were estimated visually from Weissenberg photographs, taken with CuK radiation by means of the multiple film technique.

The y and z parameters of barium were found from a Patterson synthesis based on the $0kl$ data. A two-dimensional Fourier analysis, using signs of the reflections calculated from the barium contributions alone, gave a clear resolution of the four sulphur atoms. After successive refinements, the electron density map shown in Fig. 1 was obtained. The barium and sulphur parameters are:

	Ba	S_I	S_{II}	S_{III}	S_{IV}
y	0.093	0.190	0.101	0.090	0.283
z	0.136	0.285	0.382	0.446	0.502

The reliability factor $\Sigma||F|_{obs} - |F|_{calc}|/\Sigma|F|_{obs}$ for the $0kl$ reflections is 15.4 %.

Fig. 1 shows that the tetrathionate ion possesses an unbranched chain structure, the distances $S_I - S_{III}$ and $S_{II} - S_{IV}$ in the projection being 3.17 Å and 2.85 Å, respectively, *i.e.*, too large for bonds to exist between those atoms.

This is the first structure determination for a salt of tetrathionic acid.

1. Foss, O. *Acta Chem. Scand.* 6 (1952) 802.

Received December 20, 1952.

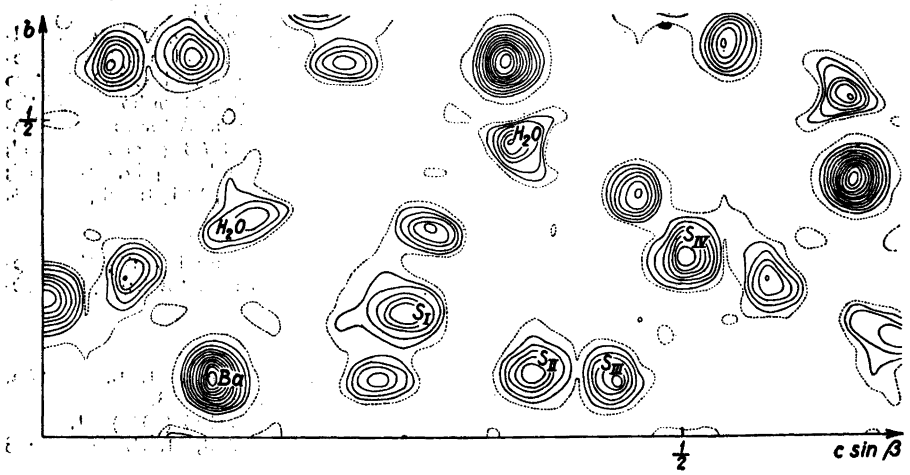

Fig. 1. Projection of $BaS_4O_6 \cdot 2H_2O$ along the a axis. The 4-electron line is dotted. Contour intervals: 10 e.Å^{-2} for the barium atom, 4 e.Å^{-2} for sulphur atoms, and 2 e.Å^{-2} for oxygen atoms and water molecules.