

Welcome to Participants

BY THE PRESIDENT OF THE UNION PROFESSOR N.V. BELOV

It is my privilege to greet you, to welcome participants in this meeting in the name of the International Union of Crystallography and to permit myself some introductory remarks. We live in the age of computers. They have not been built for us but we are allowed to use them within satisfactory limits. Notwithstanding that they are very expensive, none of us or our students wish now to compute even the most elementary of our problems with slide rules and Beevers–Lipson strips. We are all impressed by such miracles as reliability coefficients, sometimes less than 4%, but not everyone, even those interested, understands that this does not reflect the reliability of the structures themselves but only the measure of convergence of the tests of calculated and experimental intensities. The computer can give us of the order of nine significant figures whereas the experimental intensities are much less precise. Sometimes, for special reasons, they are far from correct. This means that a structure with a small R may on occasions be a wrong one – which is a pity not only for the scientist concerned, but for science as a whole. Although the production of the best program for use on a computer may sometimes be beyond the means of the individual X-ray crystallographer, care in the production of experimental results is his responsibility alone. To point this lesson is the aim of our meeting; it will be achieved not only by discussion here, but also by the distribution of the proceedings in a future issue of *Acta Crystallographica*.

It is my agreeable task to introduce Sir Lawrence, but I cannot refrain from some introductory words about the creator of Crystal Chemistry. His role is well known to everyone. I remember my own impressions of the first Russian lecture on Bragg's early results which was given by my beloved Professor Joffe during September of 1914. But, for me, the importance of Bragg's achievement is the creation of the crystallography of silicates, which has turned out to be the only true chemistry of silicates, the basis of mineralogy and petrology, indeed the basis of all geological sciences and also of the synthetic chemistry of ceramics, cement and so on. It is a pleasure to work along the lines of the crystal chemistry of silicates in such studies as that of the magmatic history of the earth's crust.

The critical point in laying the foundations of the crystal chemistry of silicates was the establishment of the structure of pyroxenes, especially of diopside, made by Sir Lawrence with his young pupil Professor Warren. The crucial point in this structure was the precise measurement of intensities. The structure was solved and the atomic parameters were determined by the aid of the Fourier method, this being its first application to the structure of pyroxenes.

And so, it is particularly appropriate that our first speaker will be Sir Lawrence.

The Early History of Intensity Measurements

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There could be no more important subject than intensity measurements for a conference dealing with our methods and techniques. It is a curious feature of X-ray analysis that there are two points in the course of the investigation when it comes, as it were, to a focus. The first is the finale of the experimental measurements which are summed up in a list of values of $F(hkl)$. All the experimental effort and cunning has gone to making these values as accurate and extensive as possible, and they represent the raw material on which the whole analysis is based. The second is of course the list of atomic coordinates, in which again a set of

numbers constitutes a full account of all that the investigator has succeeded in establishing. They sum up the outcome of the research; the answer to what he has been seeking is embodied in the 'model'. The tangle of optics simplifies itself in these two principal planes, related by each being the transform of the other.

When I received the very kind invitation to give an opening talk, I proposed to Arndt that I might give some account of intensity measurements in early days. They formed the basis of the very first determinations of structure, though in so primitive a form. The curious