Meeting Report

Vth Polish School of Crystal Structure Analysis. Trzebieszowice, 18–29 September 1976.

In view of crystal structure determination becoming routine, at least in the case of moderately complicated and well behaved structures, special consideration is now given to the other frontier topics in crystallography. Several such topics (the reliability and accuracy of crystal structure analysis, non-Bragg diffraction effects and the crystallochemical interpretation of structural data) were selected as the main subjects of the Fifth Polish School of Crystal Structure Analysis. The School was organized by the Polish Committee of Crystallography and the Institute for Low Temperature and Structure Research of the Polish Academy of Sciences.

About 100 participants from different Polish scientific centres interested in X-ray and neutron crystallography attended the School.

The scientific programme covered some main topics of interest in today's crystallography.

The theory of the symmetry of modulated structures, including the precise definition of symmetry operations and the analysis of modulated crystals by X-ray diffraction methods, were presented by Professor P. M. de Wolff, (Technische Hogeschool, Delft) and Dr J. Warczewski (Cracow). The lectures were supplemented by several examples of modulated structures and the corresponding diffraction patterns showing the satellite reflexions. Professor A. Guinier (Université de Paris-Sud) devoted one of his lectures to the small-angle scattering of X-rays and neutrons and showed some specific possibilities of both these methods. His following lecture demonstrated neutron inelastic scattering as a powerful method for the examination of lattice dynamics especially in the vicinity of phase transitions, and his final lecture discussed diffuse scattering in alloys. Diffraction of X-rays by phonons in crystals was lectured on by Dr R. Kubiak (Institute for Low Temperature and Structure Research, Wrocław). The comparison of X-ray diffraction, which 'sees' an instantaneous state of the crystal, and neutron diffraction, which depends not only on the positions of atoms but also on their dynamics, was made in the lecture by Dr J. Leciejewicz (Institute for Nuclear Researches). These problems were closely connected with the lectures given by Professor H. Jagodziński (Universität München) who gave a mathematical treatment of diffuse scattering due to disorder in crystal structures and presented qualitative and quantitative interpretations of this phenomenon. Experimental determination of TDS by application of X-ray diffraction and also by Mössbauer absorption was presented by Professor E. Wölfel (Technische Hochschule, Darmstadt).

The structure analysis of several ferroelectric crystals (KDP, TGS, SbSI, $BaTiO_3$ and Rochelle salt) in connexion with their phase transitions shows that in spite of steady progress in this field the results obtained cannot supply a satisfactory explanation of the mechanism of the phase transitions. As followed from lectures given by Dr K. Itoh (Hiroshima University), the possible origin of this difficulty comes from the nature of ferroelectric phase transitions involving small atomic displacements especially near the Curie point as well as order–disorder and anharmonic thermal motion of atoms.

Inorganic crystal chemistry and the periodic system of elements were the subject of the lectures presented by Professor N. V. Belov. The difficulties in the methods and the instrumental problems of X-ray diffraction measurements were analysed by Professor D. M. Kheiker (Moscow Institute for Crystallography) and Dr J. Grochowski (Jagiellonian University) in the lectures on improving the accuracy and economy of data collection.

Very interesting problems in the prediction of ionic structures on the basis of ionic radii and physical properties were developed by Professor F. Hanic (Slovak Academy of Sciences, Bratislava). He also considered investigations of crystal structures in extreme conditions of pressure and temperature.

Some questions from the field of organo-sulphur compounds which possess significant biological activities were presented by Dr A. Kálmán (Hungarian Academy of Sciences). The lecturer made an attempt to classify S–N bonds in terms of their length.

A few lectures were held on several further interesting problems, such as: temperature effects in X-ray crystallography (Professor K. Łukaszewicz, Institute for Low Temperature and Structure Research, Wrocław), the statistical treatment of results in structure analysis (Dr Ł. Lebioda, Jagiellonian University, Cracow), extinction effects and accuracy in structure analysis (Dr M. Cygler, Polytechnical High School, Łódź) and correction methods for absorption effects (Dr A. Stepień, University Łódź).

The School produced an occasion for many scientific contacts and interesting discussions. Two poster sessions organized during the School presented a review of the previous year's results obtained in different Polish scientific centres.

The Sixth Polish School of Crystal Structure Analysis will be held in 1979. It is intended to make this School more international by also inviting participants from other countries.

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