Meeting Report

The Third European Crystallographic Meeting. Zürich, Switzerland, September 6–10, 1976.

Over 400 crystallographers from 28 countries gathered in Zürich for the Third European Crystallographic Meeting on September 6–10, 1976. The two previous meetings in this series were held in Bordeaux, France, 1973 (Coppens, 1974) and in Keszthely, Hungary, 1974. The primary theme in Zürich was consideration of the systematic principles of inorganic and organic crystal structures, which together accounted for eight of the twelve orally presented sessions and 75 of the 116 papers given in poster sessions. In addition, sessions were held on biological crystal structures, on alloys, on non-diffraction methods and on the role of crystallographers in industrial laboratories. Seven plenary invited lectures were presented.

The extraordinary richness of chemical and structural diversity exhibited by metal phosphides with formulas ranging from M_3P to MP_{15} was discussed by H. G. von Schnering (Stuttgart). The phosphorus atom arrangement, determined by X-ray diffraction, varies from isolated atoms to open chains, infinite helices, six-membered planar rings, convex polycyclic molecular groupings and infinite one and two-dimensional arrays, with color that varies from black through orange and red to yellow. In the other plenary lecture on inorganic systematics, P. B. Moore (Chicago) made extensive use of a theorem of enumeration devised by G. Pólya in 1937, together with graph theory and combinatorials, to derive complete inventories of families of structures with formula $M_n\varphi_m$, where M represents one or more metal atoms and φ one or more closely packed anions. Among the advantages of enumerating trees of related structures are identification of 'parent' structures from which many others derive and also prediction of several very densely packed octahedral arrangements, the transition metal salts of which may have interesting magnetic properties.

The plenary lecture on systematic organic structural crystallography by A. Vaciago (Rome) explicitly recognized the second basic theme at Zürich, the societal aspects of crystallography. He emphasized the need to separate chemical crystallography into analytical and structural divisions, the former being a chemical service activity, the latter continuing as a full research activity that leads to systematic studies and understanding and that maintains high standards for the analytical work. Vaciago developed his viewpoint in terms of similar attitudes contained in the recent National Research Council report *Status and Future Potential of Crystallography*. Sten Samson's (Pasadena) lecture was a tribute to the pioneering work of Fritz Laves on complex alloy phases. He systematically considered the various ways polyhedra can pack together, leading to such complex arrangements as the μ, P, σ and E phases, and described α-Mn which appears to contain atoms of three different radii and three different magnetic moments as one of the most interestingly unique elemental structures.

W. Cochran (Edinburgh) discussed the power of neutron spectroscopy as a tool for determining the frequencies of the optic and acoustic branches of phonon wave vectors, in solids, especially at second-order phase transitions from which the dynamics of the transition can be deduced. An interesting sociological comment concerned the UK budget for neutron-beam research, which in 1975 was a total of £6.8 million for all locations. A. C. T. North (Leeds) gave an overview of the principles, at four levels of organization, underlying the structure of various classes of proteins. Both α- and β-helices are constituents of most globular proteins: the energy required to distort the peptide group from planarity is small, as is that to fold globular proteins to the conformation found in nature. The evolution of more specialized proteins appears parallel to that of the host organisms: this relation is a topic currently receiving great attention by biocrystallographers.

The remaining plenary lecture was concerned with the present and future roles of crystallographers in industry. S. C. Abrahams (Murray Hill) showed that industrial crystallographers generally use a very wide range of crystallographic techniques in problem solving. The academic education of future crystallographers must be substantially broadened to allow them to compete successfully with other physical scientists for positions in industry. The rate of production of new research and development positions in the next five to ten years, according to a recent National Science Foundation projection, will be appreciably less than the production of new PhD's. As much as 35% of all new openings for PhD's are expected to be in such non-traditional industrial areas as production and quality control, marketing, *etc.* That considerable interest was aroused by this topic was shown by the vigorous discussion following a panel discussion chaired by P. Gadó (Budapest), although consensus was not reached on the nature of the most desirable educational reforms.

The meeting format allowed unusually good opportunities for authors to interact with other participants. This was in large part because of the presentation of two-thirds of the papers in poster sessions, each of which lasted an entire day with over two hours set aside for discussion, not including the lunch interval (the cafeteria was housed on the ground floor of the meeting building). Many poster authors found that considerably more detailed and useful discussions thereby developed than is possible in oral sessions. Oral papers were given at least 20 minutes, some as much as 40 minutes. Excellent use of one of these longer periods was made by G. O. Brunner (Zurich) who showed a film simulating the two-dimensional packing of atoms. Improving on the bubble model, a closer approach to realistic interatomic force fields was obtained through use of magnets mounted at different heights, floating on an air cushion: variation of the forms and strengths of the magnets, the available area and the frequency with which the air stream was chopped gave representations of different crystal structures, defect arrays, rearrangements at phase transitions and lattice vibrational modes. In one of the 20 minute papers, P. Murray-Rust (Stirling) derived interesting correlations from the Cambridge files by means of factor analysis.

Panel discussions were held on the development of crystallographic data files, several of which were on display. An open meeting of the IUCr Teaching Commission was well attended.

This report has benefited from the comments of Dieter Schwarzenbach.

Nearly all the papers presented at this meeting have been given in the form of long (three page) abstracts, and the resulting 458 page *Collected Abstracts* are available, for SF 25, postpaid, from: ECM-3, Institut für Kristallographie, ETH-Zentrum, 8092 Zurich, Switzerland.

S. C. ABRAHAMS

Bell Laboratories
Murray Hill
New Jersey 07974
USA

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Reference

Coppens, P. (1974). *J. Appl. Cryst.* **7**, 312–313.