

MEETINGS

Eighth Congress of the International Union of Crystallography

Last August the Eighth General Assembly and Congress of the International Union of Crystallography met for the first time in the US since 1948. The plans for this meeting, as described by Walter C. Hamilton in his PHYSICS TODAY article (August, page 23) were novel and ambitious.

Here we present two views of the congress. Lyle Jensen reports the scientific highlights, and Richard Marsh examines the way the meeting was organized in the hope that the experience gained may be of value to those engaged in planning future conferences.

Highlights of the Scientific Program

The program was divided among the State University of New York College at Buffalo, SUNY at Stony Brook, and Brookhaven National Laboratory. The biological crystallographers met in Buffalo one week before the general sessions at Stony Brook. A series of two or three day topical meetings, mostly at Stony Brook, followed with the neutron diffractionists gathering at Brookhaven. The outstanding event at the biological meeting was an account of the solution of the insulin-molecule structure, completed only a few days previously. At Stony Brook, the highlights included unusual coordination in silicon, a new lattice diffusion theory, superconductors with high critical temperature, the accuracy of structure determinations and the crystal structure of polymers.

Dorothy Hodgkin (Oxford) presented the climax of a long and difficult effort to solve the structure of insulin at the Buffalo meeting. She made the first crystallographic studies on this important protein in 1935, before her present Oxford team of co-workers was even born and when only a "solution in principle" to a structure as complex as this was possible. A full solution came closer to reality two decades later, when the theory and techniques of heavy-atom isomorphous derivatives for solving the phase problem were developed. By these means, the structures of myoglobin and hemoglobin were solved, although insulin remained intractable.

The root of the difficulty lay in the fact that two heavy-atom derivatives isomorphous with the native protein crystals are usually necessary to solve the phase problem, and only one could

be prepared for insulin. Recently, a second derivative became available and, along with improved diffraction equipment, led to the solution of the insulin crystal structure. It is noteworthy that x-ray anomalous-dispersion measurements contributed significantly in this process. Knowledge of the structure of insulin should lead to a better understanding of its biological function.

A report at Stony Brook on 6-coordinated silicon by Friedrich Liebau (Max Planck Institute, Würzburg) generated considerable discussion on the reason for the unusual coordination. Linus Pauling (Stanford) gave more weight to a balanced charge distribution, as an explanation, than to electronegativity—at least in the compound SiP_2O_7 .

A new "lattice diffusion theory" was advanced by Harry E. Cook (Ford) and Didier de Fontaine (UCLA) in a unified treatment of ordering and decomposition kinetics in multicomponent systems. "Composition-wave" instabilities were analyzed in terms of normal modes in analogy to the treatment of vibrations. The short wavelengths lead to ordering, the long wavelengths to decomposition. Roger Fourme (Orsay) and coworkers reported on cooperative ordering of electric dipole orientations in several organic structures that cause a transition to an antiferroelectric state below the critical temperature.

The discovery of a new high-critical-temperature (T_c) superconductor, falling outside the two known structure types that yield high values of T_c , was reported by Angelo L. Giorgi (Los Alamos) and E. G. Szklarz.

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The theoretical significance of the meaning of accuracy in structure determinations was treated by Durward Cruickshank (Glasgow) followed by an experimental assessment by Alexander Mathieson (CSIRO, Australia). Their views generated considerable discussion on the variable quality of structure determinations, depending on the aims of the analysis. This is a problem of the sort that arises in analysis of all physical measurements. Opinion was clearly divided on procedures for assigning weights to experimental quantities used in deriving observational equations. Some thought that weights should be modified as the theoretical model evolved; others maintained that errors in the observations should be carefully estimated as part of the experiment, and thereafter used as weights in the form of inverse variances.

The role of crystallography in polymer science was discussed by Paolo Corradini (Naples), who introduced the concept of an equivalence principle in understanding the crystal structure of polymers with a regular chemical configuration. In the crystal, the repeating chemical elements of the chain must be systematically equivalent in a conformational sense along

the chain axis. It appears to be a generalization that the conformation corresponds to minimal energy for the isolated molecule. Low angle x-ray scattering studies on the liquid phase formed on transition from the nematic (intermediate between liquid and crystalline) phase, by Claude Gravatt (Bell Labs) and George Brady (Bell Labs), show that long-range order up to 30 nanometers persists as high as 15°C above the transition, with correlation lengths of approximately 200 nanometers close to the transition point.

A major field of research appears to be opening up on chemical reaction in the solid state. Many studies reported at Stony Brook showed that initiation of reaction or phase transformation takes place at one or more defects, and that its progress is largely controlled by geometrical factors. In some cases the final product is a single crystal of another phase or of a new chemical substance, the orientation of which bears a definite relationship to that of the parent. Numerous questions were raised, and many unexplained effects were described. Considerable future activity in the area of chemical reactions in the solid state may be predicted.

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Much of this report is abstracted from material submitted by the organizing or presiding chairmen of the eight simultaneous sessions. I gratefully acknowledge these contributions.

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An Experiment in Congress Organization

The form of the congress was an experiment in organization, designed to maximize the desirable aspects of a large scientific meeting and minimize the objectionable ones. For the benefit of those planning large meetings, I want to give a frank report of the successes and failures of the experiment.

During the planning stages of the congress, the steering committee anticipated that attendance figures would be in the range of 2500-3000 participants. However, budget cuts in the US and the continuing scarcity of travel funds for foreign scientists combined to reduce the final total to approximately 1500, almost equally divided between US and foreign participants. In addition, about 400 nonparticipants accompanied the scientists.

A primary objective of the program committee was to steer the scientific sessions towards a limited number of specialized, "frontier" topics, the session chairmen being given wide latitude in their selection—or solicitation—of papers that would be presented in person. Papers that were not selected for presentation, or that did not fall comfortably into any frontier topic, would appear only in the printed abstracts. Actually, nearly all of the submitted papers ended up by being presented in person.

Two factors led to this change in format: first, the number of submitted abstracts was substantially smaller than anticipated; second, most contributors pointed their abstracts towards one of the frontier topics, even if their subject matter was only

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