

CRYSTALLOGRAPHERS OFFER MEETINGS WITHIN MEETINGS

The Eighth Crystallography Congress, meeting this month in the US, offers every type of communication from crowded formal sessions to spontaneous gatherings by handfuls of specialists. Electronic communications will help participants get the most out of the meeting.

WALTER C. HAMILTON

THE US PLAYS HOST again this month to the General Assembly and Congress of the International Union of Crystallography after an interval of 21 years. The program and structure of this, the eighth meeting, reflect the broad interdisciplinary character of crystallography. Biological crystallographers have their turn first at Buffalo (see box on page 25 for meeting schedule) for a topical meeting on biologically important substances. This specialized meeting is followed by ten days at Stony Brook, during which many small meetings-within-meetings will be held on "Frontier Topics of Crystallography" (see *PHYSICS TODAY*, July, page 117 for list). More specialized symposia follow at Stony Brook and at the Brookhaven National Laboratory, and the meeting is topped off by a tour of scientific laboratories in the Washington, D. C. area.

Best of both worlds

The organizing committees have attempted to provide a program that combines the advantages of large and small meetings with few of the disadvantages of either. The structure of the program around the frontier topics and ad hoc informal sessions and the physical arrangements, which include a computerized network for personal messages and program updating, are among the more unusual features of the meeting. Special events and exhibitions in Stony Brook and Buffalo are

detailed in the accompanying boxes.

Since their beginning in 1948 the triennial general meetings of the International Union of Crystallography have grown, both in numbers of participants and papers, in a hyperlinear fashion (table, page 27). As the meetings have grown, more and more crystallographers have expressed concern about the seeming decrease in the real scientific value of alternative types of meetings: rapporteur sessions, as in Cambridge 1960 and Rome 1963, or a number of simultaneous sessions of weakly related short papers. The first challenge faced by the international program committee (chaired by George A. Jeffrey of Pittsburgh) was: "Encourage rank-and-file participation in the congresses, but produce a program structure that makes for a scientifically exciting meeting."

Another overwhelming problem of large meetings is the frequent difficulty of making specific personal contacts and arranging for quick informal discussion among like-minded scientists. The problem is aggravated when the meetings are spread over a number of hotels with perhaps one central notice board that few people ever consult. Thus challenge number two, this one for the US organizing committee (David P. Shoemaker, MIT, chairman), was: "Facilitate personal contact and ad hoc discussion among a couple of thousand individualistic crystallographers of all sorts

of interdisciplinary persuasions."

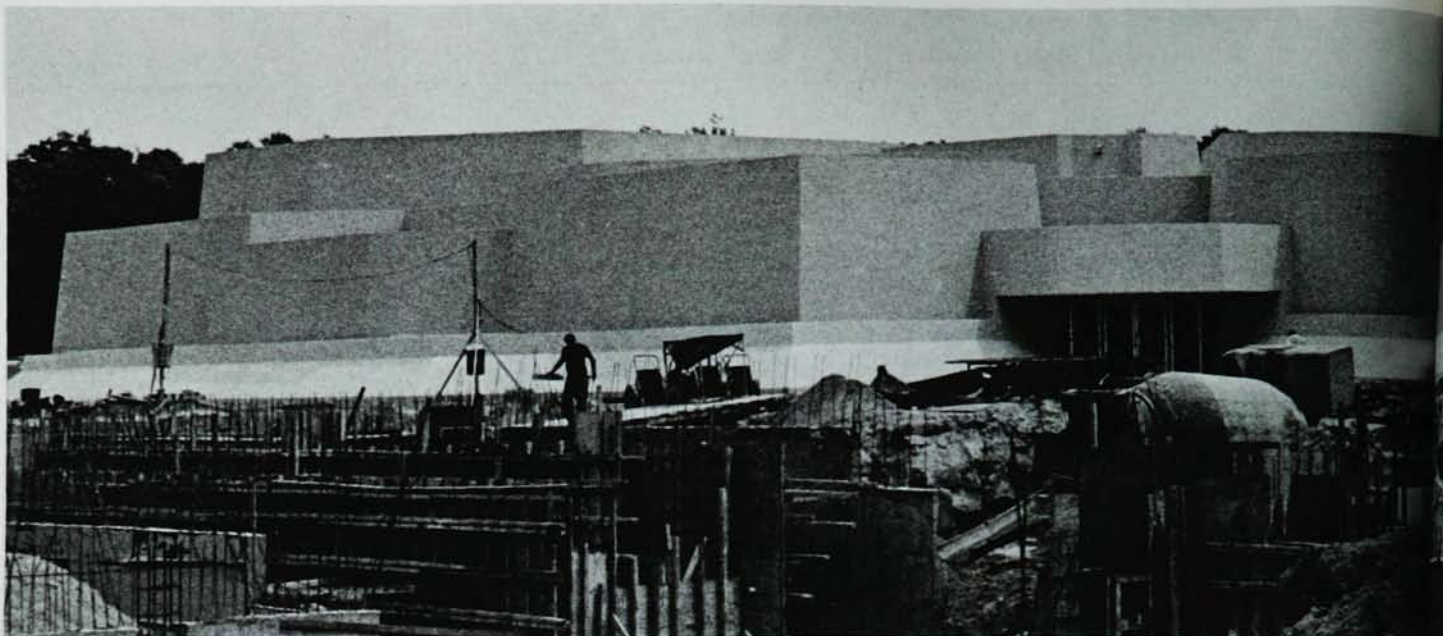
The problem for the US steering committee was to help the scientist obtain the satisfaction that usually accompanies the small (100-participant) specialized research conference (a Gordon Conference, for example) in the midst of such a large group.

Why a large meeting anyway?

When these problems were raised in preliminary discussions among US crystallographers, the skeptics re-



Walter C. Hamilton received his BS from Oklahoma State University, spent a year at the Federal Institute of Technology in Zurich, and then completed work on his PhD in chemistry at California Institute of Technology. After a year at the Mathematical Institute at Oxford, he went in 1955 to Brookhaven National Laboratory, where he is now senior chemist and deputy department chairman. He is the author of *Statistics in Physical Science* and the co-author (with J. A. Ibers) of *The Hydrogen Bond in Solids*.



STONY BROOK. Construction scars surround new lecture hall, where many of the special events and exhibitions will take place during the congress.

sponded: "Why bother? Just eliminate the large meetings, and we will all be better off." The large international meetings do allow periodic contacts among the international scientific community engaged in the varied activities that constitute crystallography. Of the 1500 registrants for this congress, 900 come from 36 countries outside the US. Many interests are shared, but the shades of different development of emphasis and interest in different countries provide fertile ground for new interdisciplinary growth—if the meeting format allows it.

Furthermore, in the case of IUCr, much union business is transacted by official delegates sitting in the General Assembly, which coincides with the scientific congress. An opportunity also exists for lengthy working sessions of the 18 union committees and commissions.

The USA National Committee for Crystallography, which represents the National Academy of Sciences as the adhering body to the union, thus has tried to construct a meeting to prove that large meetings can be great meetings.

What is crystallography?

The scientific program of a meeting should at its best represent what the science is today. Crystallography, as any science, may be defined as what

crystallographers do—or, perhaps even more, what they talk about. Thus the abstracts submitted to the 1969 congress must represent what crystallography is today, as defined by crystallographers. The 700 abstracts received before the 15 March deadline have been published in a volume of collected abstracts, which has been distributed to participants and which has been also issued as a special supplement to *Acta Crystallographica*,

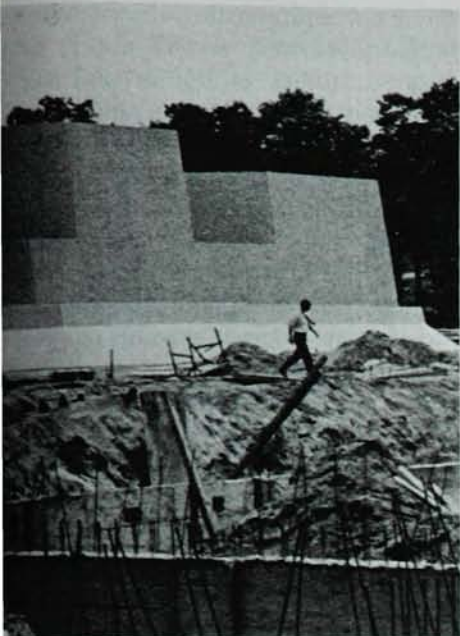
Part A. This volume thus serves as our definition. (Those not attending can order copies of the collected abstracts from Polycrystal Book Service, Box 11567, Pittsburgh, Pa., 15238 for \$15 as long as the supply lasts.)

It was clear from the beginning, however, that oral presentation of all the material in the abstracts would result in the traditional, stifling sessions of long sequences of short papers. The program committee thus decided

PHOTO BY WILLIAM GRAHAM



CHAIRMAN. George A. Jeffrey, chairman of the international program committee, confers in Washington with Elizabeth A. Wood, a member of the steering committee.



SPECIAL EXHIBITIONS AT STONY BROOK

Commercial Exhibit—Earth and Space Science Building
Crystallographic and allied equipment. 13–16 Aug.

Noncommercial Apparatus—Lecture Hall Building
Gadgets and one-of-a-kind instruments constructed by scientists. Will run the length of the Stony Brook meeting.

Photographic Exhibition—Lecture Hall Building
Photographs of crystals and of diffraction patterns of crystals chosen more for their esthetic than their crystallographic interest. Will run the length of the Stony Brook meeting.

Book Exhibit—Lecture Hall Building
Books and journals of interest to the crystallographer. Organized by Polycrystal Book Service.

Films—Physics Auditorium
Scientific films with crystallographic themes. Will be shown at frequent intervals throughout the congress.

to begin by asking the questions, "What are the really active areas in crystallography today? What are the 'frontier' topics?" The committee polled the international crystallographic community and asked national committees and distinguished individuals from many countries to make suggestions. More than 100 suggestions were received, out of which the program committee selected about 50 topics for emphasis.

Announcing these topics in advance polarized the contributed abstracts. Many authors carefully emphasized the relevance of their results to a particular topic. Key words, which form the subject index of the collected abstracts, rendered such recognition easy. The overall effect was less that of a shotgun assortment of papers than has obtained at previous congresses. Whole groups of papers were aimed at a particular frontier topic. The abstracts were often more informative than in the past, and one cannot help concluding that competition for a place in the program was a factor. To some extent this result defeated the original intent to reduce the number of papers presented. Many chairmen argued for two sessions rather than one half-day session on the grounds that the papers were too good and too relevant not to be heard. For example the session on lattice dynamics and thermal motion grew into a two-day meeting within the meeting.

Chairmen's mandate

The formal part of the Stony Brook program consists of individual ses-

sions, each of which corresponds to one of the frontier topics. Each session will occupy a half day or a full day; cochairmen have been given complete freedom in planning their session. Their mandate was, "Construct a great three-hour program on your topic. You may use the relevant abstracts that have been submitted or use other source materials and speakers, according to your judgment."

Thus the chairmen were charged with arranging a session of exciting science—not just sorting and arranging contributed papers. In many cases the chairmen have strengthened their programs with invited lectures—not necessarily represented in the abstracts. In other cases, one keynote lecture will be followed by contributed papers, chosen from among those abstracts most relevant to the topic. In a few sessions all those who submitted abstracts to the chairmen will be given the floor.

Speakers are asked to talk only on the main subject of the frontier topic, although their abstract may contain other factual information. This restriction should reduce the temptation to flit from session to session to pick up a particular paper and is designed to encourage audience participation. The program committee hopes that the frontier-topic discussions will be of interest to most crystallographers and not only to those intimately involved in the topic. Thus the format should encourage the growth of interdisciplinary work.

Judging from their expansion into more than one session, the topics with

EIGHTH CONGRESS OF THE INTERNATIONAL UNION OF CRYSTALLOGRAPHY

Calendar

7–12 AUGUST

State University College at Buffalo. Topical meeting on crystallography of biologically important substances

13–21 AUGUST

State University of New York at Stony Brook. General assembly and frontier topics

22–24 AUGUST

Stony Brook. Topical meetings: Dynamical diffraction, small-angle scattering, solid-state reactions, crystal morphology

22, 23 AUGUST

Brookhaven National Laboratory. Chemical and physical aspects of neutron diffraction

25–27 AUGUST

Washington. Laboratory tours

Special events

7 AUGUST

Buffalo. Congress opening. Alexander Rich speaks on "Crystallography of hydrogen bonding in purines, pyrimidines and nucleic acids"

13 AUGUST

Stony Brook. Linus Pauling, "On the importance of being crystallized"

22 AUGUST

Brookhaven. John Axe, "Dynamical effects in phase transitions," Martin Blume, "Magnetization density in solids", E. F. Bertaut, "Representation analysis," and P. Heller, "NMR and neutron-scattering measurements of magnetic critical fluctuations."

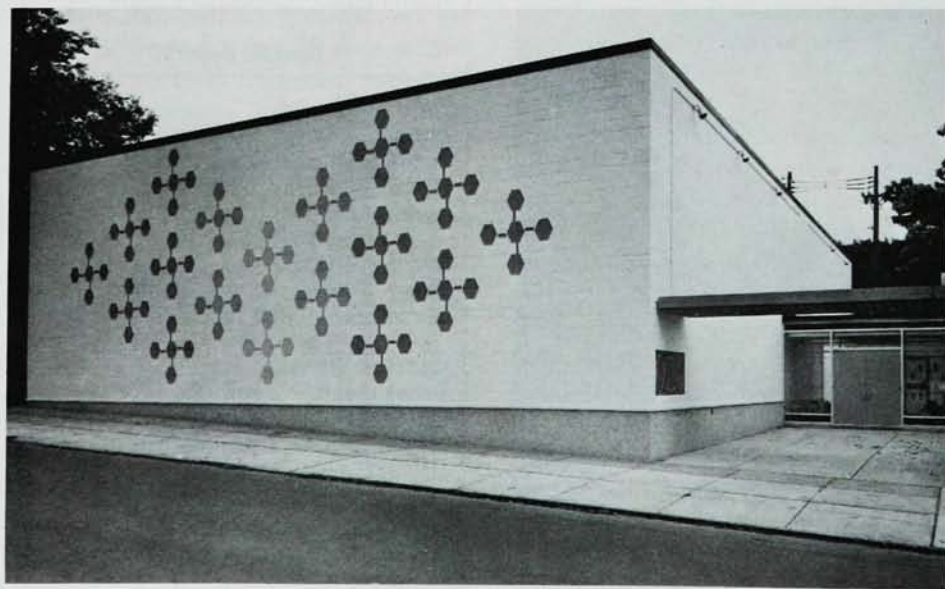


US NATIONAL COMMITTEE. Planning the congress are, from the left, William Parrish, secretary of the US committee; David P. Shoemaker, chairman of the US organizing committee; Walter C. Hamilton, Stony Brook local chairman; Sidney C. Abrahams, a delegate to the congress; Benjamin Post, steering committee member; and William Zachariasen, a member of the executive committee of the International Union of Crystallography.

PHOTOS ABOVE AND CENTER BY WILLIAM GRAHAM



MORE COMMITTEE MEMBERS. Listening intently are, from the left, William C. Kehl, secretary of the American Crystallographic Association; Kenneth Hedberg of the US National Committee; Robert A. Young of the steering committee; Richard E. Marsh, an alternate delegate; and Bertran E. Warren, a vice-president of the IUCr.



BUFFALO. The Center for Crystallographic Research, directed by David Harker.

the most enthusiastic followings are: lattice dynamics, crystal optics, diffraction studies of liquids and solutions, systematics of inorganic structures, conformation problems and steric interference effects in organic structures, instrumentation for high intensities and high and low temperatures, and growth structure and properties of thin films. An especially timely paper, and possibly a real sleeper, is the paper by William Parrish and Nathan Spielberg on "Instrumentation for X-ray Analysis of Returned Lunar Samples" to be presented in the session on phase identification and data representation.

Topical meetings

Some suggested special topics appeared to have enough coherence and current interest to demand more comprehensive treatment than would be possible in a half-day frontier-topic session. These subjects have been designated for topical meetings that will not only treat problems at greater length but will also be more like symposia among experts.

Of the topical meeting in Buffalo, David Harker of the Center for Crystallographic Research says, "I think we shall have, in Buffalo, the most spectacularly successful meeting on biologically important substances the world has even seen. The quality of the abstracts indicates that the papers will be fantastic." Opening the session are two papers on the crystallography of transfer RNA—one of the most exciting problems in biochemistry today. More than 20 papers discuss structural investigations of proteins in varying stages of refinement, several to a resolution of better than 0.3 nm.

The topical meeting at Brookhaven will include working sessions on new techniques in neutron-scattering experiments. Other key topical meetings are being held at Stony Brook following the frontier-topics portion of the congress, and in addition the frontier-topic session on lattice dynamics and thermal motion has grown into a two-day meeting-within-a-meeting.

Ad hoc sessions

When scientists assemble it is inevitable that like minds will want to get together to discuss particular topics not covered in the scheduled sessions and to continue discussions that were terminated in the regular sessions because of time pressure. For such ad hoc meetings, additional rooms are

Past Congresses of the International Union of Crystallography

Year	Site	Number of participants	Number of papers
1948	Cambridge (USA)	310	83
1951	Stockholm	340	173
1954	Paris	630	385
1957	Montreal	600	282
1960	Cambridge (UK)	1200	417
1963	Rome	1300	514
1966	Moscow	3200	831
1969	Stony Brook	— ¹	700 ²

1. Because of the recent recession in science funding, which applies all over the world but is particularly severe in the US, the large attendance at Moscow in 1966 will not be repeated at Stony Brook in 1969.

2. Number of accepted abstracts.



CONGRESS SYMBOL HONORS A.L. PATTERSON

The official emblem of the Eighth International Congress of Crystallography is the planar projection of what has come to be known as the Patterson synthesis. Arthur Lindo Patterson, in his classic paper on the structure of potassium dihydrogen phosphate (*Z. Krist.* **90**, 517, 1935), introduced it, calling it simply the F^2 synthesis:

$$P(x,y,z) = \sum_h \sum_k \sum_l \frac{1}{V^2} |F(hkl)|^2 \cos 2\pi (hx + ky + lz)$$

where F is the structure factor; h , k and l the Miller indices of the reflecting planes; x , y and z the coordinates in Patterson space; and V the volume of the unit cell.

The Patterson diagram portrays systematically the vectors between all pairs of scattering centers (atoms or ions) in the structure, weighted with the associated product of their scattering powers. The positions of these vectors relative to each other are unknown. In the Patterson synthesis they are given a common origin. The contours in a Patterson diagram show the density distribution of the scattering powers at the ends of the vectors.

Because it contains all the information obtainable from the Bragg reflections of the crystal, the Patterson synthesis is a powerful first step in the solution of nearly all crystal structures. If it can be fully interpreted, the structure is solved. Commonly it makes possible the determination of the positions of the heavy atoms which, in turn, leads to a complete solution of the structure.

Introduction of the Patterson synthesis was a giant step forward in crystal-structure analysis. Lindo Patterson also enriched the roster of known crystallographic structures, especially in the field of biologically important substances. Working at the Institute for Cancer Research near Philadelphia, where his widow, Elizabeth, does research in biophysics, he trained many young people in crystallographic analysis. He died in Nov. 1966.

He was one of the founders of the American Crystallographic Association, an author of the constitution of the International Union of Crystallography and a major contributor to the *International Tables for X-ray Crystallography*.

being provided. Several frontier-topic chairmen have anticipated the need for additional discussion periods. Any group may arrange for a room with or without projection facilities during the Stony Brook meeting. A number of such rooms already has been reserved by groups who knew in advance that they wished to have sessions on topics not included in the formal program. The program committee considers the ad hoc sessions one of the more unusual aspects of the meeting; future program chairmen will be watching the results closely.

Rapid communications

The ad hoc meetings are the most experimental part of the congress. If they are to succeed, attracting participants (other than those who have set up the meetings) at the last moment, the entire congress must be notified of the times, places and subjects. A system of remote terminals connected to the central Stony Brook computer will make this notification possible. Announcements of ad hoc meetings and other changes in program will be fed into a central computer file. Congress participants at 12 key campus locations—including the lecture and dining halls—will be able to obtain an updated printed program for the day simply by typing a request into the computer terminal. Periodic revisions of the program obtained from the terminals will be posted in these locations. The same system will help solve the other problem of large conferences—the difficulty of contacting other participants. Each preregistered attendant has been assigned a number. Messages telephoned to the central station will be placed in a computer file identified by the participant's number. At any one of the terminals a simple request will cause the stacked messages for that participant to be typed out.

Washington tour program

When the Stony Brook portion of the congress is over, about 100 congress participants will tour the Smithsonian Institution, National Bureau of Standards, Goddard Space Flight Center, National Institutes of Health, Geological Survey and various university laboratories in the Washington area. A flexible program is planned, in which participants will be able to talk with scientists in the various laboratories. We expect that this part of the program will be most popular with first-time visitors to the US. □