

CRYSTALLOGRAPHY

THE SIXTH CONGRESS

AND ASSOCIATED SYMPOSIA

By *I. Fankuchen*

The Sixth General Assembly and International Congress of the International Union of Crystallography, which convened in Rome during the period from September 9 to 18, 1963, was a far cry from the first Congress of the Union which was held at Harvard University from July 28 to August 3, 1948. The Union actually had been founded two summers earlier at a conference held in London in 1946. The first and sixth meetings form an interesting study in contrasts. At that delightful first Congress, there was a total of about 85 papers presented, including a few invited addresses. Everyone gave his own paper. Actually, there was ample time for this personal presentation. While there were some joint sessions, these occurred only on two mornings of the six-day meeting and the conflicts were not serious. By way of contrast, at the Sixth Congress there were somewhat more than five hundred papers grouped under 21 different topics and at times as many as five simultaneous sessions. Another aspect of the most recent Congress, one which markedly influenced its general character, was the almost universal application of the rapporteur system. This system had been initiated three years earlier at the 1960 meeting in Cambridge, England, and, while it had been only partly successful there, it had been hoped that the experience gained in Cambridge would lead to a more successful application of the rapporteur system at the larger meeting in Rome. Alas, these hopes were not realized. After having faithfully attended every session possible, this reporter felt that scientifically the meeting was almost a complete loss as far as he was concerned. No paper, as discussed by a rapporteur, made a vivid impression

on him. It is unfortunately true that the use of the rapporteur system removes any personal contact between the author of a scientific work and the audience. There was naturally a wide range in the quality of the reports by the rapporteurs; some of them quite obviously had not taken their assignments seriously and did poor jobs. A few had worked very hard but, despite their most valiant efforts, the impact of the research being described could simply not come through.

There were also abuses of the rapporteur system. At one session the rapporteur had the contents of seven papers to present and seventy-five minutes in which to do it. He used thirty minutes to report on five papers then announced that the sixth paper had such a good abstract that he didn't have to say anything about it! He used the remainder of the time on a complete discussion of his own paper, the last of the seven. Although the chairman of this session did not stop him, she rectified the situation beautifully. Upon completion of the rapporteur's account she stood up and announced that inasmuch as paper No. 6 had only been read by title the author would now be given ten minutes to present it himself. Loud applause greeted this well-deserved rebuke.

The attendance at the Congress was good—almost too good. About 1500 crystallographers attended the meeting and this, of course, made it somewhat difficult to find specific people with whom one wanted to talk. Almost everyone one wanted to meet was in Rome—except for the East German crystallographers, who, for some unexplained political reasons, were not able to come. Some Americans also did not attend the meeting—apparently in a rather silent protest of the decision to use the rapporteur system. It seems to be more and more generally felt that the rapporteur system must be eliminated or, at the very least, appreciably modified.

It was hard work if one took the meeting seriously. Three social events lightened the grind of rapporteur after rapporteur: a most delightful

I. Fankuchen is professor of applied physics at the Polytechnic Institute of Brooklyn. His account of the 6th General Assembly and International Congress of the International Union of Crystallography in Rome is amplified in the following pages by separate reports on three symposia held in connection with the Congress and on an open session of the Union's Commission on Crystallographic Apparatus. The reporters are G. A. Jeffrey (University of Pittsburgh), Gabrielle Donnay (Carnegie Institution of Washington), David R. Chipman (AMRA, Watertown Arsenal), and S. C. Abrahams (Bell Telephone Laboratories, Murray Hill, N. J.).

chamber music concert by I Musici, a cocktail party sponsored by the Philips organization in a real castle, the Castel San Angelo, and the Congress dinner at the spectacular new Hotel Hilton.

Two aspects of the continued development of x-ray crystallography emerged fairly clearly as a result of the Rome meeting. One is the fact that the wide-scale use of high-speed computers has now made it possible for x-ray crystallographers to dare to tackle structure determinations of very complicated substances with the expectation of being able to arrive at complete structures. Most crystals apparently can now have their structure determined if one is willing to spend enough time and money on the job. Concomitant with the use of computers is the need for better data-collecting mechanisms, particularly for the complicated large unit cell structures now being studied; and so the other aspect of the development is the emergence of automatic data collectors, some involving the coupling of digital computers and x-ray apparatus, others the construction of analog computers as part of the x-ray equipment.

If, for this reporter, there was a highlight to the Rome meeting, it was the report by H. C. Watson of the work that the Cambridge (England) group is doing on myoglobin. For one of the early workers in this field, it is quite exciting to see, as the years pass, the slow unfolding at higher and higher

resolution of this almost impossibly complicated crystal structure. It really looks as though it is now coming out.

Two very valuable adjuncts to the meeting were the magnificent instrument exhibits and the book exhibit. Both of these were extremely well done and appreciated. At times it looked as though more people were examining the instruments and books than attending the lectures.

At the meetings of the General Assembly the usual business of the Union was conducted. Two new members were accepted: Hungary and Pakistan. The next Assembly will be in Moscow in 1966. The International Union of Crystallography will probably add to its already large publishing program two new items: a new journal devoted to applied crystallography and a book of reproductions of Escher's beautiful symmetry drawings.*

The main meeting was followed by three symposia: I. Problems and Methods in Crystallographic Computing; II. Phase Transformations in Solids; and III. Some Aspects of Lattice Dynamics. In addition, the Commission on Crystallographic Apparatus held an open meeting in which automation was the major topic under discussion. The following reports deal individually with each of these events.

* *The Graphic Works of M. C. Escher*, Duell Sloane and Pearce, 1961.

I. *problems and methods in*

CRYSTALLOGRAPHIC COMPUTING

By G. A. Jeffrey

Forty papers were presented in two and one-half days at the symposium on problems and methods in crystallographic computing, and this was a welcome change of pace from the rapporteured sessions of the previous week. With a few exceptions, the papers were concerned with programming for various aspects of crystal-structure analysis. General-purpose machines were invariably used, ranging from the IBM 1620 class to the ATLAS at Manchester.

From crystallographic laboratories throughout the world, programming methods were described to deal with every stage of the research, from controlling the instrument that collects the "raw" experimental data to presenting the results in a stereochemically comprehensible manner.

For some time it has been thought that there are no longer any unsurmountable obstacles to a fully

automatized structure-solving system that could tackle most crystal-structure problems. The symposium further enhanced this belief, but in fact still left it unproven. What may be holding back the development in most countries is the lack of resources available to the crystallographer, because it has become obvious that computing at this level of sophistication is going to be very expensive. The discussions of the more general solutions of the phase problem, for example, all presupposed ample time on a computer of the IBM 7090 class or greater. From this point of view, the part of the conference concerned with programs for the smaller machines consisted of a series of intellectual exercises in "making do with what was available."

The most desperate need for full automation was in the application to protein structures, where the very large number of observational data and