

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.

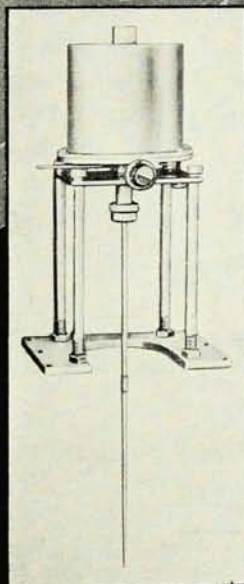
For some time it has been thought that there are no longer any unsurmountable obstacles to a fully

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



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atomic parameters makes any human participation in the calculations very tedious. If solving protein structures were as important as reaching the moon, this problem could be solved rather quickly. However, with such a small fraction of most national

resources devoted to basic research, it seems likely from this conference that the crystallographers in the world may have to continue exercising their programming ingenuity on undersized computers for some time to come.

II. PHASE TRANSITIONS

By Gabrielle Donnay

Of the forty papers contributed at the symposium on phase transitions, nine unfortunately came after the deadline and thus will not appear in the printed abstracts. The symposium was divided into eleven sessions, three of which were devoted to invited one-hour lectures.

The first of the invited papers, presented by M. J. Buerger of the Massachusetts Institute of Technology, preceded the symposium. Its purpose was to survey the advances made in the field and perhaps to intrigue members of the Congress into staying the first three days of the following week to learn more about the subject. I believe Professor Buerger succeeded on both counts. He showed how his structural classification of transitions into reconstructive and displacive ones overlaps the thermodynamic division into first and higher orders, and he suggested that mixed transitions may occur that involve both types of orders.

R. A. Young of the Georgia Institute of Technology spoke of his own detailed study of the mechanism of the quartz transition at 573° C, which entailed, among other things, refined structure determinations at eight temperatures below and above the transition (R indices less than 4%).

A. R. Ubbelohde of Imperial College, London, pointed out the need for just such careful single-crystal observations during phase transitions. He discussed the phenomena to be looked for, among

them coexistence of multiple domains of slightly different structures, on the one hand, and continuous slight changes of one-crystal structure that remains homogeneous throughout, on the other.

These three lectures provided the stimulation that comes from hearing about an interesting subject from experts with different backgrounds and different ways of looking at the same phenomena. Thus, even without contributed papers, the symposium would have been a success.

As it was, many of the contributions illustrated the points raised by the invited speakers; others brought out new ones. The Russians are very active in this field and had eight interesting papers. Among them were the following: a new classification of magnetoelectric properties (seven in all), NMR studies of ferroelectric phase transitions, and a study of ferroelectric-antiferromagnetic transitions that accompany *compositional* changes in solid-solution series. This latter type of phase transition, which is of particular interest to mineralogists, has attracted little attention so far in this country.

The attendance at all sessions was surprisingly good, considering that even the most enthusiastic crystallographer must have been close to saturation by then. The general appreciation of this symposium is evidenced by present plans to hold another symposium on the same topic *before* the next IUCr Congress in Moscow in 1966.

III. *some aspects of*

LATTICE DYNAMICS

By David R. Chipman

Because of the proximity of the International Conference on Lattice Dynamics in Copenhagen from August 5 to 9,* Symposium III of the Rome meet-

ing in September was designed, not as an opportunity for presentation of the latest results in the field of lattice dynamics, but rather as an elementary course to give the average crystallographer an understanding of the types of problems which

* See *Physics Today*, February 1963, p. 102.