THE IUCr INTERNATIONAL CONGRESS

By K. N. Trueblood

THE fifth triennial International Congress of the International Union of Crystallography was held in Cambridge, England, from August 15 through 24, 1960. In addition to nearly 450 general papers classified under 19 different headings, there were 5 general lectures on different specialized topics, a panel discussion on the theory of metals, and two symposia. The first symposium had some 36 contributions concerning thermal motion in crystals and molecules; the second consisted of about 100 papers dealing with lattice defects and the mechanical properties of solids. Abstracts of all contributions, including the symposia, will appear soon as an issue of *Acta Crystallographica;* most of the abstracts indicate where detailed publication is planned. Eight of the Russian contributions appeared in an issue of *Kristallografiya* (Vol. 5, No. 4, 1960) which was distributed at the congress.

As with all international organizations, the meetings of the IUCr are plagued with the problem of exponential growth. Attendance was greater by about one power of 10 than that at the initial meeting in Cambridge, Massachusetts, in 1948, and exceeded expectations by more than 50 percent. During the first week alone, there were more than 1200 participants from 30 countries, and more came especially for the symposia, held August 20–24. The number of papers was about 50 percent greater than that at Montreal in 1957.

The fact, although not the magnitude, of this flood had been anticipated by the program committee, which had therefore introduced the rapporteur system for dealing with general contributions under what they deemed to be the most probably over-crowded topics. Ideally, the rapporteur, himself an expert in the field and an able and forceful speaker, presents a critical review of a number of related papers, emphasizing not only the salient points of each contribution but also perceiving and tracing over-all threads and trends. The authors of each paper reviewed, who have supposedly submitted informal manuscripts to the rapporteur two months earlier, are in attendance, and after the rapporteur's review there is an equal amount of time devoted to general discussion. During this period, authors can clarify or briefly elaborate on points which they feel have been given inadequate emphasis.

When the plans for using rapporteurs were first announced they caused almost universal misgivings and some acrimony; the most sceptical remained away and so presumably remain totally unconvinced. However, many, although not all, of those who came to Cambridge as doubters felt that on the whole the system worked remarkably well. Everything depends upon the selection of the rapporteurs. Eighteen different people were used in this capacity at Cambridge, covering between them some 45 percent of the general papers (all of those under the headings of minerals, metals and alloys, inorganic structures, organic structures, and proteins and related compounds). They had an average of 11 papers each to review, in an average time of slightly more than one hour (including time for discussion). It sounds like an impossible assignment, but with surprisingly few exceptions they did an outstanding job. There was no doubt that the best did more for many of the papers than could the authors themselves; furthermore, the need for simultaneous sessions in these very popular areas was greatly reduced.

Among the objections voiced concerning the rapporteur system, in addition to the obvious one that the presentation is not by the person most familiar with the work, were that it makes it impracticable to transfer from one session to another because the rapporteur almost necessarily regroups the papers in his session and cannot follow a rigid schedule, and also that it depersonalizes too much, preventing the audience from becoming acquainted with the authors. Offsetting these difficulties, however, are the saving of about two-thirds of the time which the papers would require by the normal scheme, so that many fewer simultaneous sessions are held and consequently less running back and forth is necessary, and the fact that the authors can, and usually do, participate in the discussion following the rapporteur's presentation. Furthermore, the objectivity and detachment of the rapporteur often acts as a useful filter for the audience; the rapporteur can point out the forest, with the author arising later to draw attention to those particular trees which are his favorites. I attended eight of the eighteen rapporteured sessions and heard first-hand reports of four of the others, and came away convinced that the advantages significantly outweigh the defects. The system could profitably have been used in a number of additional sessions as well, including some parts of the symposia; there are still some authors who feel it helpful to show thirty-odd slides in a dozen or so minutes. Of course one inevitable problem of the system is the need for a great deal of preparatory work on the part of the rapporteur, particularly when his papers cover a considerable variety of topics; for this meeting an average of two to three weeks of full-time digestion of manuscripts and literature was required. And of course the chief reward of an outstanding presentation is the opportunity to perform again if the system is retained.

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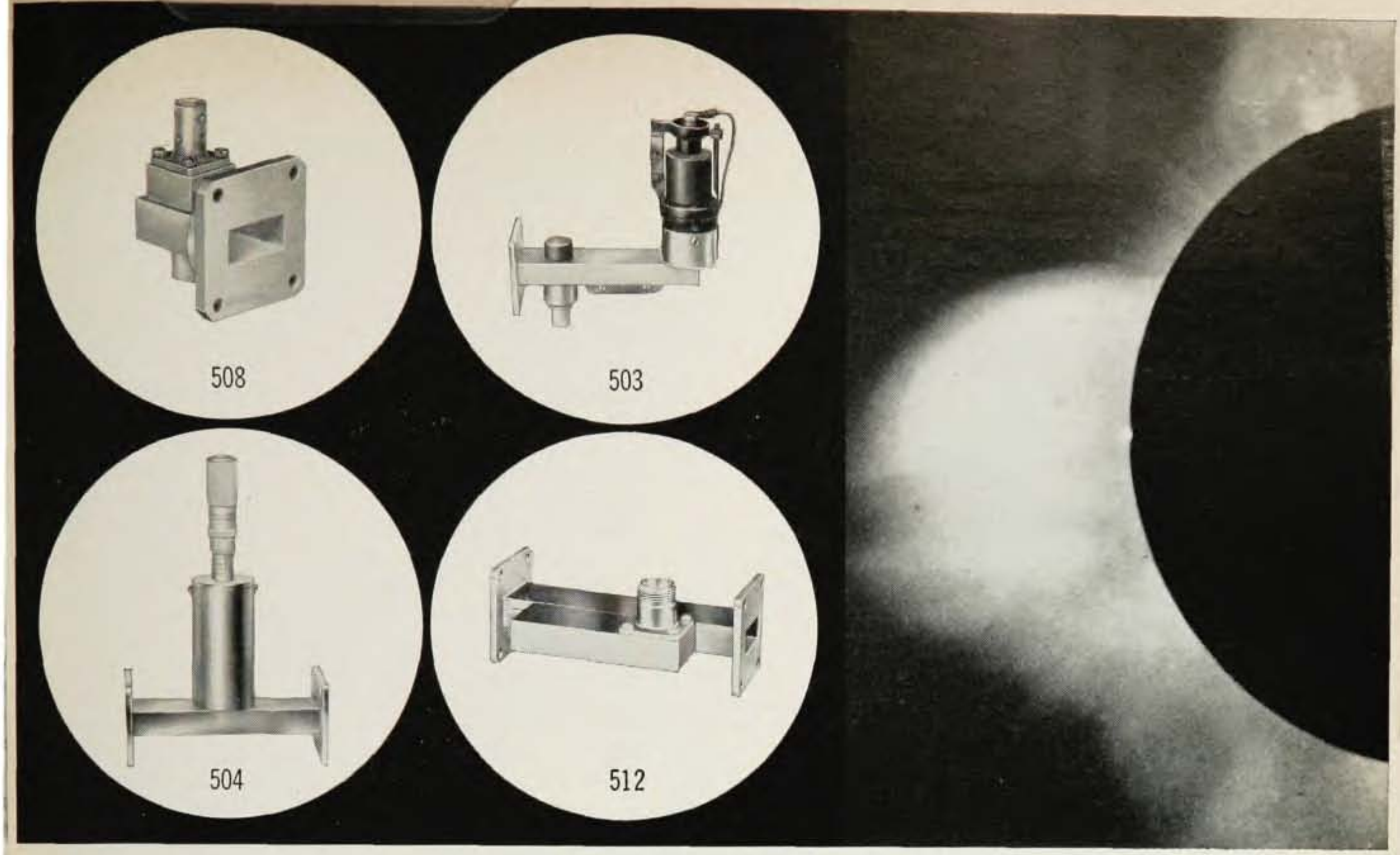

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ONE of the much-anticipated highlights of the congress, a scheduled three-sided discussion between N. F. Mott, J. C. Slater, and L. Pauling, on the theory of metals, was robbed of some of its sparkle by the absence of Professor Pauling, who remained in the USA because of the imminence of his engagement with the Senate Subcommittee on Internal Security. However, R. Rundle, with the aid of D. P. Shoemaker, did an extremely effective job of presenting the advantages of Pauling's resonating valence-bond theory, while agreeing with Slater that such empirical approaches would be unnecessary when quantum mechanical calculations on real metals become practicable.

In other general lectures, N. V. Belov gave a clear and well-illustrated account of recent progress in the crystal chemistry of the silicates, especially in the USSR; J. H. Van Vleck presented a beautifully lucid discussion of magnetic alignment; M. F. Perutz spoke on the structure of crystalline proteins, with of course especial emphasis on the remarkably fruitful work of his own group on hemoglobin and of Kendrew and his collaborators on myoglobin; W. L. Bragg reviewed, as he is almost uniquely qualified to do, the growth in the power of x-ray structure analysis from 1912 to the present; and B. K. Vainshtein discussed the theory and practice of direct methods of structure analysis, with emphasis on work in the USSR. The two symposia were introduced with general lectures by Slater and Mott.

No effort will be made here to review either these general lectures or the detailed papers. It is clear that one can now expect a continually increasing emphasis in structure analysis on the chemistry and physics of the arrangements found, rather than merely on their geometry. This is a natural consequence of the steady progress in methods of solving unknown structures and the increased precision which has resulted from the better data and the greatly improved refinement techniques of the last five years that are now used almost routinely. For suitably rigid molecules, one can now derive from x-ray or neutron diffraction data approximate descriptions of the translational and librational motion in the crystal; for other molecules one may, with more ambiguity, be able to say something about internal torsional oscillations or even in some cases internal vibrations. For simple molecules the latter can be studied with precision in the gas phase by modern electron diffraction methods, and the results, when coupled with spectroscopic data, can yield an improved description of the intramolecular potential function. X-ray studies of solid-state reactions, or of crystalline intermediates in reactions normally occurring in other phases, are becoming more common; typical of the latter are the many studies, in more than a half-dozen different laboratories, of complexes between metal carbonyls and hydrocarbons or related materials. Similarly, studies of complex crystalline hydrates and of substances which occur in different tautomeric forms in the solid state and in solution are providing additional clues concerning the nature of solutions.

Of course the most remarkable structures discussed at the meeting are those of (sperm-whale) myoglobin and (horse) hemoglobin which have been solved entirely by direct methods involving as many as seven different isomorphous substitutions. The close relation of the structures of these molecules not only to those of similar proteins in other species but even to each other has profound implications. At present the hemoglobin molecule has been "seen" only at about 6 A resolution, while the Fourier synthesis of myoglobin has been extended to 2 A. About one-third of the side-chains in myoglobin have already been identified with certainty and another third tentatively, far in excess of expectation when the electron-density synthesis was calculated; data to extend the resolution to 1.2 A will be available shortly. For hemoglobin, the ultimate limit of resolution will be about 1.8 A, so that although most individual atoms will never be resolved, most of the constituent amino acids will probably be identifiable. The contrast between the labor involved in these studies and that now required for the most favorable structure analyses of relatively simple structures cannot better be illustrated than by pointing out that it took just as long (three weeks) to build a scale model of the myoglobin molecule, which contains an intricately folded and coiled chain of 153 amino acids, as to carry out an entire structure determination, from first photo to final refinement, of crystalline catechol, $C_6H_4(OH)_2$. The latter tour de force was accomplished by C. J. Brown; of course he had a favorable case with stable, easily formed crystals and a planar molecule. On the other hand, he had only a relatively slow computer available; he might have saved three days with a very fast one.

The General Assembly of the IUCr chose P. P. Ewald to succeed J. Wyart as president until the next Congress and Assembly, to be held in Rome in the summer of 1963. Smaller meetings on selected topics will probably be held in Tokyo in the autumn of 1961 and Munich in 1962, the latter to celebrate the 50th anniversary of the discovery of the diffraction of x rays by crystals.

Within the limitations imposed by the confines of Cambridge, the arrangements for the meeting were all that could be expected. Overseas visitors particularly appreciated the receptions and college dinners, the many trips arranged both in Cambridge and in its environs, and the superb orchestral concert of 17th to 20th century English music given in King's College Chapel by the Philomusica of London. Unfortunately many of the meeting rooms were not large enough for the sessions so that it was sometimes impossible to get in if one had not arrived on time. Closed-circuit TV helped greatly to alleviate this difficulty during the symposia; some indeed preferred to watch on TV, where they could hear far better and often see the slides and blackboard better, although they had no opportunity to participate in the discussion because two-way circuits were not available. The meeting was supported in part by funds from UNESCO and some 50 industrial and scientific organizations; the IUPAP helped in the organization of the second symposium.