

Meeting Reports

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The XIIth Congress of the IUCr, Ottawa, August 1981. An informal report

Since its formation in 1947, the International Union of Crystallography has held its Congress and Assembly regularly every three years in various parts of the world. The list of venues for the past half dozen occasions is impressive: Cambridge (UK), Rome, Moscow, Stony Brook (USA), Kyoto, Amsterdam, Warsaw. This time it was Canada that invited the crystallographers. The National Research Council of Canada hosted the Congress in Ottawa at Carleton University campus.

We report first on the affairs of the Crystallographic Union; then on the scientific meeting.

One of the essential tasks that the Union must perform on these occasions is to elect its officers for the next three-year term. The new President of the Union, elected at this Ottawa meeting, is Dr Jerome Karle (of Washington, USA), widely known for the fundamental role he has played, over the past twenty years, in the development of direct methods for the solution of crystal structures. The new Vice-President is Professor S. Ramaseshan (of Bangalore, India), known for his contributions to crystal physics. The new Secretary–Treasurer is Professor K. Kurki-Suonio (of Helsinki, Finland). This latter post is one of particularly challenging responsibility, as will now be explained:

The Union came to a significant crisis during the past year, as a matter of fact. This was a financial tumble, which is now past history but which has left us in a somewhat injured condition. When the Union started up, in 1947, it was a very much smaller, simpler, more manageable thing than it is now. From the start, it was a publishing body, producing *Acta Crystallographica*; but the world's financial climate was steadier than now, and the Union's actual expenses were quite light, for *Acta Cryst.* ran to only 400 pages per year. Since those days, the number of crystallographers has increased by an order of magnitude (it is now 8000); the science itself has become vastly more productive; the volume of our published material runs to about 5500 pages each year and, to handle this publication business, there is a staff of half a dozen full-time employees in an office in Chester. Moreover, the activities

of the Union are international. The Union's income (mainly subscriptions to the Journals) comes in from all over the world. As with any other international operation, the Union is financially vulnerable, being affected unavoidably by major currency fluctuations, particularly in the relative value of the pound sterling and the Danish krone, and it was this which, during the past year or so, caused the trouble referred to at the start of this paragraph. Details are complex, and cannot be spelt out here, but the principal consequence of this recent experience is a loss of financial reserves, and the postponement, for at least one year, of our acquisition of in-house typesetting, which, up till very recently, had been the fully agreed and widely welcomed intention. Such was the nature of our recent crisis.

These financial matters received considerable attention during the meetings of the Assembly in Ottawa. To avoid any further damage from currency fluctuations in the future, the Union is making a number of administrative adjustments. In particular, printing costs will be incurred in the same currency as that in which subscriptions are collected and, to monitor the cash-flow situation, two new committees have been set up. The first of these, a *Finance Committee*, will keep a continuous watch over the Union's financial position and its reserves. The members of this body will be the President (or Vice-President), the Secretary–Treasurer, the Chairman of the Journals Commission and two or three other members, of whom two will be Professor Michael Woolfson and Professor Durward Cruickshank. The second new committee is a *Long Range Planning Committee*; this will meet less frequently but will have a correspondingly wider remit. These two new bodies will considerably assist the new Secretary–Treasurer in his task.

Turning now to the scientific program of the Ottawa meeting, the considerable size of these three-yearly events requires some emphasis. At this Congress, about 1300 crystallographers took part, plus about 200 accompanying persons. They represented a total of 40 different countries – of which the first nine were (in order of the numbers present): USA (400), UK (140), Canada (120), West Germany (100), France (70), Japan (60), Sweden (50), USSR (50) and Switzerland (35). To these statistics one has to add the impressive weight and volume of the scientific program: 7½ full days of working sessions, comprising 12 main lectures, 890 poster presentations and 220 oral contributions, as well as the formal

meetings of the official Commissions and, of course, those of the Assembly itself. The successful organisation of this large mass of scientific activity was achieved by the use of a combination of two techniques: parallel oral sessions, usually five each morning, and, each afternoon, a display of about 180 poster presentations. The total number of abstracts to be read was over 1000. Parallel sessions force conference members to make invidious decisions but the device is essential nowadays for coping with the number of oral sessions that are needed to cover the wide scope of modern crystallography. As for the other device, the poster presentation, this is so much an established and successful feature of crystallographic conferences now that it is hard to believe that 'posters' were a completely new thing for us only a little more than ten years ago. Nowadays it would be almost impossible to stage any major crystallographic meeting without them. Poster presentation has a number of real merits in addition to the time-saving aspect; crystallography is a subject rather well suited to it, and many poster presentations these days are works of considerable skill, ingenuity and craftsmanship.

What can be said of the content of all these different presentations? What's new in crystallography? This is a hard question to answer in a limited space. There were some excellent main lectures. Especially popular were those relating to biological topics, and those on materials science. In the latter category, that given by Dr R. E. Newnham (Penn. State) was an eye-opener in regard to the extraordinary advances of crystal engineering in the fabrication of ever smaller, faster, and more complex crystal-based electronic circuits and devices. In the former category, the lecture by Sir David Phillips (Oxford) was outstanding, including a motion picture of an animated lysozyme molecule, in computer-calculated thermal motion. Two other particularly memorable main lectures were those by Professor F. Hirshfeld (Rehovot, Israel) on charge density studies and Dr P. Murray-Rust (Stirling, Scotland) entitled 'Crystals, Molecules and Chemists'. Under the auspices of the Teaching Commission, two particularly useful review lectures were presented: on the place of crystallography in modern science, by Professor B. K. Vainshtein (Moscow) and on the applications of crystallography to materials science, by Dr S. C. Abrahams (Bell Telephone Laboratories, USA). The first of these related our specialised subject to the

whole spectrum of scientific disciplines, from pure mathematics through chemistry, physics, biology, geology and engineering, with numerous up-to-date examples. In the second, the creative role that crystallography can perform was illustrated by a series of examples from research done in Bell Laboratories, featuring not only analyses and quality testing but also the design and characterisation of new solid-state materials.

It is, of course, quite impossible to summarise the contents of 1000 separate contributions but we may note certain trends, and make a number of observations. Papers and posters had been contributed to the meeting organisers in terms of a scheme of formal headings, set out systematically in the preliminary circulars of the congress and intended to cover virtually all currently active areas of crystallography. The responses under these headings were remarkably uneven and it is of interest to note where emphases occurred. Considering the poster presentations only, for simplicity, there were a great many more or less straightforward structure determinations: 120 under the inorganic/mineralogical headings, 130 under organic/organometallic. Evidently, the determination of new structures is still a major activity of crystallographers, over the world. Equalling these two traditional areas (and much surpassing them in sheer volume of diffraction data) came structural molecular biology (125 posters). Next in popularity came biochemical/pharmaceutical topics (70), with phase transitions and structure-property relationships running close behind (65) and 'real' crystals (*i.e.* defect studies) about equal (70). By contrast, apparatus and techniques attracted only 20 posters, symmetry-related topics 30 and electron diffraction studies about 20. (Computing accounted for 45 contributors and neutron diffraction for 15; but there had been a Summer School on Computing and a Symposium on Neutron Diffraction just prior to the Congress.)

Among several special topics that stood out, giving this meeting its 1981 flavour, was that of *synchrotron radiation* (SR). Besides being the specific subject of one of the main lectures (by A. B. Stuhmann), it turned up repeatedly in other places. SR is, possibly, the first thing to mention in answer to the question, 'What's new?'. It is, of course, not merely a source of very high intensity X-rays but it has the additional feature of wavelength tuneability which renders it invaluable for EXAFS (see below). Besides that, it is an ideal tool for

maximising anomalous scattering for phase and chirality determinations. Here and there, among poster presentations of protein work, where sample diffraction photographs were routinely on display, one would frequently notice an outstandingly crisp, clear picture; looking more closely one would find it to have been obtained with SR, and the exposure time given was, typically, of the order of three minutes. EXAFS (*extended X-ray absorption fine structure spectroscopy*), mentioned above, is another 'new' entry on the crystallographic scene – new enough still to require a fresh *ab initio* explanation each time it is talked about. It is an effect complementary to diffraction. There is no doubt as to its value, at least for the exploration of the immediate environment of (particularly) selected metal atoms within a protein molecule. Furthermore, very new indeed, within this area, is the application of EXAFS to *single* crystals in controlled orientations (although one could remark that this is really rather an obvious development, when one recalls the excellent plane-polarised character of SR). A pretty convincing application of this to Hans Freeman's plastocyanin, only months old, and not yet quite fully worked out, was enthusiastically shown by Professor K. O. Hodgson (Stanford).

With the mention of proteins, we must return to comment again on *biological structures*. The Ottawa meeting was characterised by a tremendous wealth of reports of work on proteins, and protein systems of many kinds, viruses and membrane structures. Many different protein refinements were described, often to 2.5 Å resolution, some using up to 20 000 structure amplitudes; some refinements included neutron diffraction data; in many cases there were very detailed identifications of solvating molecules (and anions) around a protein; there was detailed mapping of hydrogen bonding, and discussion of proton mobilities. Meanwhile, the Protein Data Bank was exhibiting its services; solved protein structures, having atomic coordinates deposited in the Bank, now number approximately 175. The progress made in this whole area during the past decade or so is enormously impressive.

These observations lead us to another point, which is connected with the subject of publications and the nature of our journals. The presence of so many rather broadly based studies, such as those on biological systems, at the Ottawa meeting, contrasts rather strongly with the current pattern of our journal, *Acta Cryst.*, Section B. One might expect essentially

the same proportions of such broad-based topics, relating biological function, or, for that matter, chemical or physical properties of substances, or groups of substances, to underlying structural principles. In fact, our journal does not, at present, carry many articles of this kind, either on biological systems, or chemical, or mineralogical or other large areas of physical science. This is a pity; however the Commission on Journals is aware of this defect and is taking steps to correct it. The decision to split off the category of short, compact crystal structure reports so as to form a new Section of *Acta Cryst.* had already been taken at the Warsaw Congress (1978). At Ottawa, this decision was confirmed, and it is now timetabled to begin with the January 1983 issues. From that date, *Acta Cryst.* will appear in three Sections, A, B and C. The new Section C will contain all crystal structure determinations for which there is a minimum of discussion. Section A will deal with the foundations of crystallography, including all new methods, or theories (and their initial exemplification). Section B will become, in effect, a new journal in its own right, based on the traditions of the present Section B, but with much wider horizons and greater depth: it is intended to contain papers on all aspects of structural science – chemical, biological, mineralogical, *etc.* *JAC* will remain unaffected by these changes. It is the hope of the Journals Commission that this new development will go some way towards reflecting the true position of crystallography as one of the central sciences of our time.

The activities of the Congress were not wholly business or scientific exchanges, of course. There were numerous sight-seeing trips. There was the main Congress excursion to a big wooded picnic site where, from reeking charcoal braziers, 880 superb beef steaks were served out with professional expertise. The Canadians had also arranged a number of exhibits: minerals; scientific postage stamps; crystallographic plane groups in Canadian-Escher idiom... and, particularly impressive and beautiful, a display of graphic art inspired by and/or embodying liquid crystals: the work of D. Makow of the NRC. Our hosts had also been imaginative in their selection of souvenirs for members of the congress: the carrier bag, for instance, hand-made by Eskimos and decorated attractively with the pleasing red and white maple leaf tetracluster (Congress emblem); and, more technically interesting, even valuable, was the sheet of paper each participant was given, bearing two minute

[diameter 152(5) μm] spheres of single-crystal ruby, all ground from the same initial raw material source and available for each crystallographer to use as a well characterised reference standard, in his or her own laboratory.

One of the unforgettable events of the Congress was its Opening Ceremony. We shall remember the huge Arts Centre, its cavernous interior studded with 1000 lights; an audience of nearly 2000; the statesmanlike address, *avec parties d'importance en Français*, given given by the NRC President, Dr Larkin Kerwin, emphasising that what we need today is not so much a policy for science but rather, science within our policies; and the Canadian songs, both English and French, sung by the very professional Cantata Singers of Ottawa. Further, we shall remember the fascinating discourse, 'Insulin in Crystals', delivered by Professor Dorothy Hodgkin and, most unforgettable of all, those dramatic moments when, alas, under the heat of the fierce illumination that the projectionists were using, some of her slides jammed and even melted (yes, while projected on to the immense 40 ft screen, one of them liquefied in full view of the audience!), a pitiful indignity, which was borne by Dorothy with all her inimitable good humour and charm. Finally, we shall also recall the special message, formally read out by President Kato, that had been received from that father-figure of modern crystallography, Professor P. P. Ewald, who now (at 93) was just a little too immobile to be able to attend the meeting in person. Ewald, who was himself a key figure in the founding of our International Union, and was the first Editor of *Acta Crystallographica*, added to his good wishes the reflection that 'only through world-wide peaceful cooperation is a thorough understanding of our science to be achieved'.

J. H. ROBERTSON

School of Chemistry
University of Leeds
Leeds LS2 9JT
England

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Commercial exhibits and data base displays at the XIIIth Congress and General Assembly of the International Union of Crystallography

Scientists attending the XIIIth IUCr

Congress in Ottawa had a unique opportunity to examine and compare some of the latest, most powerful diffraction instrumentation available to them from commercial manufacturers. They could also evaluate the scope and utility of four structural data bases by hands-on demonstrations *via* computer links that in one case spanned the Atlantic. The site of most of these displays was an ample 4700 square-meter area in the main hall and foyer of the Carleton University Centre – a well-marked stop on the walking route from the Commons Building to the several lecture rooms and poster areas used by the Congress.

The Cambridge Instruments Canada Inc./Enraf-Nonius, Nicolet/Syntex, and Siemens AG exhibits each featured fully automated single-crystal diffractometers with complete, tested software packages. The Rigaku Corporation had brochures available describing a similar system. Nicolet, Rigaku and Siemens also offered associated sets of structure-determination and refinement programs that could be run with the same dedicated computer used for diffractometer control and data collection. The Nicolet system, with programs based on *SHELX* (Sheldrick, 1976), was in operation at the exhibit and could be used by visitors with appropriate input data. Huber Diffraktionstechnik GmbH displayed a single-crystal diffractometer suitable for automation; their representatives had additional information on hand that described the larger instruments currently being adapted for synchrotron-radiation experiments.

Versatile automated powder X-ray diffractometers were highlights of the Philips, Stoe/California Scientific Systems, Rigaku and International Business Machines displays. Several systems offered sophisticated software packages for profile analysis and/or phase identification *via* programmed searches of standard pattern files. Elaborations of one such set of programs were presented by IBM scientists at a poster session (Parrish & Huang, 1981; Huang, Ayers & Parrish, 1981). This simple method of augmenting and advertising commercial exhibits might well be emulated by others at future meetings.

Newly developed instruments in the field of position-sensitive X-ray detectors were shown by Marconi-Avionics, Stoe/CSS and Technology for Energy Corp. (TEC). All devices were linear, gas-filled proportional counters, the first two achieving spatial location of signals by delay line, the third by rise-time encoding. Active lengths and claimed resolu-

tions were: 50 mm, 0.12 mm (Marconi-Avionics); 100 mm, 0.1 mm (TEC); and 130 mm, 0.2 mm (Stoe). The central wire of the Stoe detector was curved to a 130 mm radius through a novel magnetic levitation technique. Literature on a television-based two-dimensional PSD, designed from a system developed by Arndt & Gilmore (1979), was distributed by Enraf-Nonius. This device is to be integrated with the manufacturer's CAD4 diffractometer system and may not be sold as a separate entity.

Information about another (much older) kind of two-dimensional PSD could be obtained from the representatives of Ceaverken AB and Eastman Kodak Co. Products available from these vendors were part of the updated study of X-ray film characteristics presented by Dawson, Mills & Elder (1981) during the open meeting of the Commission on Crystallographic Apparatus.

Workers in diverse crystallographic disciplines have sensed a growing need for systematic computer-assisted schemes for deposition and retrieval of structural data. These needs have been addressed though the good will of small groups of crystallographers around the world who have established, maintained and improved data bases devoted to identifiable areas of structural research. A popular island among the commercial exhibits in the Unicentre was occupied by four of these systems – the Cambridge Structural Data Base, the Inorganic Crystal Structure Data Base, the Metal Structure Data Base, and the JCPDS/CIS Data Base. Coupled with information status reports on each of these files during the open meeting of the Commission on Crystallographic Data, the working displays in the Unicentre should have stirred the interest and imagination of many visitors. A fifth data base, the Protein Data Bank, was also described at the open meeting, with further information available at a table in the Commons Lounge.

Crystallographers owe a special debt of thanks to their colleagues (Olga Kennard, G. Bergerhoff, L. D. Calvert, A. D. Mighell, C. R. Hubbard, T. F. Koetzle, among others) who have contributed their time and talent to setting up these invaluable data centers.

This brief summary is doubtlessly biased by some of the particular interests of the writer, and certainly omits many instruments, X-ray generators, image processors, etc. in the exhibition that must have had special significance to others. For these oversights, the indulgence of the exhibitors must be sought. Finally, the