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INTERNATIONAL UNION OF Crystallography

NEWSLETTER

Volume 7, Number 3 ♦ 1999

Ted Baker

Thoughts On The International Union

Technically I will no longer be President of the Union by the time you read this. The Glasgow Congress will be over, the organisers will be relaxing, and the rest of us will have arrived home, inspired by the science. For me this is also a final opportunity to speak through this column and an opportunity to thank you all for the support and friendship I have received over the past three years. To serve as President of the Union has been an honour that I never imagined would come my way and it is an experience I will treasure.

I would also like to use this occasion to reflect a little on the Union and its activities. Some of these are changing radically, driven by changes in our subject, or in science and society. The pressure on subscriptions to our journals is one that is facing all print journals and the move to electronic publishing is unavoidable. Looked at another way, however, it is also an exciting opportunity that can transform how our science is presented. We are also seeing a rapid evolution in the role and importance of structural databases. These are central to the interests of crystallographers everywhere and the IUCr faces challenges in helping to ensure that these data remain readily accessible to all.

Other roles and activities of the Union remain the same, however. Of paramount importance is our international nature; it is this that defines the Union, and it is only this that differentiates us from any other national or regional scientific society. My mentor, Dorothy Hodgkin, had links all round the world, visiting, working with and encouraging scientists as far afield as China, Japan, India, Australia, New Zealand and Africa. This spirit of internationalism is shared by many in the Union and is our main raison d'etre.

There are international challenges, - how to better support crystallographers in South America, or build crystallography in Africa, or involve more Asian countries in the Union, or help with financial problems in Eastern Europe. It is also all too easy to be inward-looking, or to forget how our lives and our science are enriched by direct (not electronic!) contacts with colleagues who are far removed geographically and culturally. It is for these reasons that the issues raised by Richard Nelmes in this issue of the Newsletter are important and should be pondered. Speaking for myself, the greatest benefit that science has brought me has been the network of friends and colleagues all round the world, both in their friendship and in what I have gained scientifically. This has also been true of my three years as President, and it is what makes the "I" of IUCr so important.

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The IUCr Newsletter is distributed to 587 libraries and 15,000 crystallographers and other interested individuals in 39 countries. Feature articles, meeting announcements and reports, information on research or other items of potential interest to crystallographers should be submitted to the editor at any time. Submission of text by electronic mail and graphics, slides or photographs by express mail is requested. Items will be selected for publication on the basis of suitability, content, style, timeliness and appeal. The editor reserves the right to edit. Cost of distribution in Australia, Colombia, Croatia, Cuba, Czech Republic, France, India, Italy, Japan, Malaysia, New Zealand, Poland, South Africa, Switzerland, Taiwan, The Netherlands, Thailand, and Venezuela is borne by crystallographic associations or institutions or by individual crystallographers in these countries. Address changes or corrections and requests to be added to the mailing list should be addressed to the editorial office.

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On the Cover: The glory that was Glasgow '99, presiding President Ted Baker and President-elect Henk Schenk in kilts at the Ceilidh, Local Chair Chris Gilmore and Program Chair Judith Howard in repose with the fire extinguisher, Scottish highland daners and pipe band, and delegates enjoying scottish hospitality and viewing posters in a splendid setting.

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Letters to the Editor

Bill,

I read with interest your editorial in the latest issue of the *IUCr Newsletter*. It is unfortunate indeed when crystallographers decide (for whatever ill-conceived reason) that they are being persecuted and need to wage a holy war against some other part of the community. Your editorial reminded me of the conscientious effort made to include all facets of crystallography in the IUCr Congress in Seattle in 1996 meeting. The powder/inorganic community is hard to get to a crystallographic meeting because they tend to go to the scientific topical meetings focused on whatever they are working on at the time. The broad crystallographic community should be grateful that the macromolecular crystallographers have worked so hard to maintain a working infrastructure for the ACA and IUCr within which they have always been welcome. As you say, when it comes to organizing a meeting that attracts the broad community, the sessions chairs are the key. I don't think any group has a right to whine unless they have offered to step up and do some work and have been refused the opportunity.

Jim Jorgensen

Dear Jim,

I'm sure the macromolecular crystallographic community will be pleased by your accurate appraisal of their critically important contribution to the continued prosperity of the IUCr and its regional associates. Your comments are especially welcome coming from a recognized leader of the Materials Research and Neutron Diffraction Community.

Bill

Dear Bill,

We were delighted to see the report on last November's 'High Pressure Commission Workshop' in the latest Newsletter. But an unfortunate editing of our original text left the statement that this was "the first of the Commission's activities since it was formed at the Seattle Congress in 1996". Far from it! It is only fair to those who put in all the work of local and program organizing to record that there were two previous meetings - a one-day symposium at the international AIRAPT conference in Tsukuba in August 1997, and a three-day workshop at ESRF Grenoble in November 1997.

John Parise, SUNY Stony Brook, and
Richard Nelmes, U. of Edinburgh

Bob Gould in a Seattle nightshirt at Karaoke Night at the Seventh Intensive Course on Structural Analysis in April 1999. (photo coutesy of Leopoldo Suescun)

Polycrystal Book Service to Close in 1999

After 50 years of service, Polycrystal Book Service is going out of business. This decision is prompted by an inability to find a buyer willing to assume the operation, at any price. Polycrystal will remain in business during 1999 for the primary purpose of selling all remaining stock on hand, including two recently produced Polycrystal publications, Don Ward's Patterson Peaks and IUCr Teaching Pamphlet Number 20, Betty Wood's Crystals: A Handbook for School Teachers. Polycrystal will complete the ordering of *Acta Crystallographica* subscriptions, and turn them over to Munksgaard for future renewals. Orders and back orders still in process will be completed. Listings of remaining stock will be posted on the Polycrystal website (http://www.dnaco.net/~polybook/).

Thank you for your patronage for the past 12 years of our ownership, and for your loyalty to Polycrystal over the decades.

Mert and Wade Adams
from the ACA Newsletter, Spring 1999

Editorial

The phenomenal success of the 18th Congress and General Assembly of the IUCr is due in great measure to the tireless effort of Program Chair Judith Howard and Local Chair Chris Gilmore. We see them smiling through on the cover of this issue with a fire extinguisher ready to put out any and all fires. Chris and Judith and their friendly, efficient, enthusiastic and energetic young crew turned a meeting for 2600 people into an intimate fun-filled family affair. They have raised the standards for future meeting organizers. Nevertheless, I feel certain that local chair Joel Bernstein and program chair Martin Kaftory will rise to the occasion in 2002. This issue of the newsletter contains a serious commentary from Richard Nelmes concerning the importance of having the site of the international congresses rotate throughout the world in a timely way. Many of the delegates to the General Assembly were dismayed that the 2005 meeting will not be held in Japan. In the days following the vote to hold the 2005 congress in Florence, Italy, members of the IUCr Executive Committee discussed implementation of procedures that will assure equitable rotation of future congresses throughout the crystallographic world. The Executive Committee may have to take a more active role in setting guidelines and criteria for bids to hold future congresses. It seems obvious that by 2008 a shift of congress site to the Asian region will be absolutely essential and long overdue. I only hope that our colleagues in Japan will be willing to consider bidding once again to host the meeting. The exceptional quality and range of crystallographic research in Japan and that country's ancient and rich cultural heritage make it a most appropriate congress site.

The publication and distribution of this newsletter and the success of crystallographic meetings like the Glasgow Congress receive significant support from a core of manufacturers and distributors of crystallographic instruments, computers, software, supplies and books. Please remember to express your appreciation to these people when visiting their exhibits at meetings, when arranging to purchase their products or when you have occasion to speak with them on the phone.

The back log of meeting reports and other material awaiting publication continues to grow. The further delay imposed by the time required for printing and posting compounds the problem. The IUCr Newsletter office places the full text of each issue on the internet within 5 days of submission to the printer so that an electronic version is rapidly available. The extent to which distributing the newsletter on line could improve communication and reduce cost is being explored. Readers who would be satisfied with an electronic version could be removed from the general mailing list.

The exhibitors gathered in Glasgow for a group photograph. Their generous support and participation enhances the discipline and our meeting.

IUCr Glasgow - Remarkable in Every Way

The 18th Congress of the International Union of Crystallography in Glasgow, Scotland was the largest and most successful ever. Over 2,650 crystallographers spent nine days sharing the latest information on crystallographic theory, methods, techniques, software, hardware, instrumentation, application, data storage, retrieval, and analysis. Eight full days with six (and sometimes seven) concurrent sessions (often with standing room only) were required to do justice to the remarkable scope of the field and the extraordinary advances and productivity in all areas including crystal growth, synchrotron radiation, area detectors, *ab initio* powder diffraction analysis, *in situ* reactions of materials and biological molecules, automatic phase determination, high resolution (0.8Å and better) protein structure determination, and data mining for design of everything from rational drugs to smart materials.

At the jubilant opening ceremony, the Ewald Prize was awarded to G.N. Ramachandran for his early, enduring, and critically important contribution to the field of structural biology. M. Vijayan accepted the award on behalf of Dr. Ramachandran. Following the award, a musical program and slide show introduced the audience to the grandeur of the Scottish landscape and stirring beauty of traditional Scottish music and dance. There followed a copious feast of magnificent food in the best "tradition of Scottish hospitality" that continued throughout the entire 10 days of the meeting.

The official delegates to the congress from 37 countries spent three evening sessions attending to official Union business, the most important being reviewing the fiscal reports that show the Union to be in good health, charting future plans to insure stability and expanded activities, electing a new president, and new members of the Executive Committee and commissions and selecting a site for the 20th Congress to be held in 2005.

For the first time in memory, two candidates were proposed for the office of President. Hartmut Fuess and Henk Schenk graciously agreed to stand for election. The union will continue to enjoy the leadership and service of both candidates since Hartmut will continue to fulfill the last half of his six year term and Henk (who would other wise have left the committee) was elected to a three year term as President. M. Tanaka of Japan will serve as Vice President of the Executive Committee for the next triennium and Sine Larsen (Denmark) will continue as General Secretary and Treasurer. M.A. Carrondo (Portugal), W.L. Duax (USA), and Z. Zhang (China), were elected from a field of 6 candidates to join L.A. Aslanov (Russia), J.C.A. Boeyens (South Africa), and H. Fuess (Germany) as ordinary members of the Committee.

Very persuasive bids to host the IUCr Congress in 2005 were presented by delegations from Japan and Italy. The secret ballot in favor of holding the meeting in Florence, Italy startled many delegates who assumed that by 2005 a shift in meeting site to the Asian crystallographic community was essential to the international spirit of the Union.

The members of the Commissions of the Union organized sessions to attend to the vitally important activities of the union, setting standards, devising experiments to establish measures of accuracy and precision, planning future meetings and activities, and charting the course of the IUCr's many publications.

Reports from the chairs of the 32 plenary lectures, 97 microsymposia, and 12 commission meetings are now being filed. These reports can be viewed on the IUCr website. If reports of particular interest to you have not yet been filed, you may want to let the session chair know that you are very interested in seeing his or her report. Session titles and e-mail addresses of all chairs can be found in the meeting report file.

The Glasgow Convention Center provided a superb venue for the largest exhibition of crystallographic equipment, software, and supplies ever held. The exhibits, the poster sessions, and vendors of food and drink were assembled around an Internet Café that kept the delegates in touch with activities on the homefront while they caught up on research around the world.

A splendid evening session in honor of J. Monteath-Robertson that chronicled the growth and development of crystallography at the U. of Glasgow was preceded by a buffet of marvelous Indian food.

At the Kelvingrove Art Gallery, wineglasses in hand, the delegates viewed masterpieces, sampled splendid hors d'oeuvres, and listened to classical music provided by string soloists and ensembles. In addition to traditional masterpieces, archeological artifacts, and suits of armor, a special exhibit of whimsical African ceremonial coffins intrigued the delegates.

The highlight of the social program was the Gala Ceilidh, an evening of traditional "fayre", food, drink, conversation, music, dancing and song. The food was excellent and endless and the delegates (many of whom had rented kilts for the occasion) threw themselves into the dancing with wild abandon. The organizers had arranged a Scottish dance practice for the night before the Ceilidh and on the farewell evening an advanced course in modern Scottish rock dancing featuring a bagpipe and drum ensemble named Mac Umbra brought the house down.

The extraordinary pace of crystallographic research, the unlimited potential for new structural information arising from genome analysis, combinational chemistry, crystal engineering, and material design, guarantee that the science at the 19th Congress in Israel is 2002 will be even more extraordinary than in Glasgow, but it is unlikely that any future meeting can match Glasgow when it comes to the social program.

The Executive Committee for 1999-2001, Vice President M. Tanaka, President H. Schenk, and Secretary/Treasurer Sine Larsen (seated) . M.A. Carrondo, Z. Zhang, T. Baker, H. Fuess, J.C.A. Boyens, Malcolm Cooper, L.A. Aslanov, and W.L. Duax (standing).

Carbohydrate Binding by Proteins

A variety of proteins bind carbohydrates in order to perform the functions they are to fulfill. Some act on carbohydrates and alter them chemically, some sense the presence of carbohydrates and trigger the action of other proteins, some bind to carbohydrate in order to locate at particular sites of action, the list continues to expand. The lectins are one such group of proteins. Some bind carbohydrates with specificities that rival antibodies. They can also aggregate glycoproteins and other carbohydrate-containing macromolecules in solution and cause their precipitation (agglutination). A wide variety of plants, including the legumes and the grasses, have lectins that are distributed at varying concentrations throughout the plant, bark, foliage, fruit, seeds. Lectins are some of the earliest proteins studied crystallographically and concanavalin A (con A) and wheat germ agglutinin (WGA) are the two most prominent examples. Ironically, it is still not clear what roles lectins fulfill for the plants they serve.

The origins of affinity and specificity of carbohydrate binding by proteins have been a primary scientific goal from the earliest structural studies. Most of the fundamental factors controlling affinity were described by F. Quiocho and coworkers in structural studies of bacterial periplasmic binding proteins. Structures of carbohydrate complexes with WGA by C. Wright also made important contributions. An important recent contribution to the field is a paper by Ravishankar, Suguna, Surolia and Vijayan, "Structures of the complexes of peanut lectin with methyl-ß-galactose and *N*-acetyllactosamine and a comparative study of carbohydrate binding in Gal/GalNAc-specific legume lectins" [*Acta Cryst.* D55 (1999), 1375-1382]. Included for comparison are previously published structures of complexes with lactose and with T antigen from the same laboratory. One important conclusion is that the source of the 20-fold higher affinity of peanut lectin for T antigen over lactose and lactosamine comes not from direct protein–carbohydrate interactions, but rather from hydrogen-bond bridges to T-antigen carbohydrate from protein-bound water molecules, bridges that are not made to carbohydrate in other complexes even though structurally homologous water molecules are present. A detailed analysis of the role of water is presented and it emerges that in many cases key protein–carbohydrate interactions are fulfilled by water surrogates.

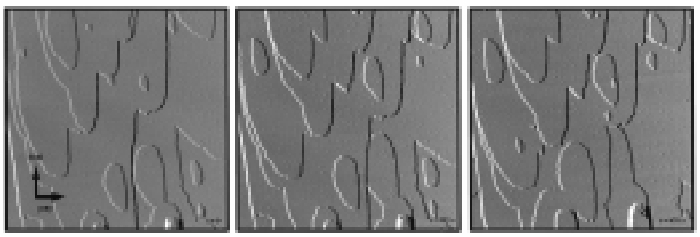
The legume lectins have a number of other curious attributes. Some show evidence of circular permutation that is the result of post-translational modification. In order to express their agglutination property, they form dimers and tetramers, but despite their relatively close homology, more than one kind of quaternary structure has been observed. In con A, favin and pea lectin, for example, six-stranded backbone ß-sheets in monomers fuse to form twofold symmetric twelve-stranded sheets in dimers, and tetramers have 222 symmetry. Not so in peanut lectin, GS4 and EcorL. In peanut lectin, six-stranded sheets in monomers are pressed together in dimers so that strands are close to perpendicular, but tetramers show neither 222 nor fourfold symmetry. The lectins have taught us much about protein chemistry over the years, but it appears we still have much to learn from them.

Howard Einspahr
Bristol-Myers Squibb Pharm. Res. Inst., Princeton, NJ USA

Unusual Layered Growth of Catalase Crystals

Atomic force microscopy (AFM) has made visible the most intimate processes of crystallization. A tiny silicon nitride micro-needle hooked to a transducer and drawn with microtome-precision and feather-weight across the face of a growing crystal can produce breathtaking images that record crystal growth at or near molecular resolution. Some of the finest examples of AFM analyses applied to questions of protein crystal growth have come from collaborations of A. Malkin and A. McPherson at UC Irvine. These include studies of lysozyme and thaumatin in which screw dislocations are imaged on growing surfaces, growth-step edges are typically one unit cell in height, and construction of individual unit cells appears to be completed before the construction of new unit cells is begun.

In a paper by Ko, Day, Malkin and McPherson, "Structure of orthorhombic crystals of beef liver catalase" [*Acta Cryst.* D55 (1999), 1383-1394], quite a different set of observations is described for the growth of catalase crystals. The observations were made on an orthorhombic crystal form of beef liver catalase rather than the original trigonal one. Salt precipitation was substituted for polyethylene glycol to remove complications to the AFM experiment without loss of isomorphism. The orthorhombic crystal structure was solved with some difficulties presented by multiple pseudo-symmetries. The unusual observations related to growth on a <110> growth face are the following. Surprisingly, no screw dislocations are observed for growth in the c direction and the face develops exclusively by two-dimensional propagation perpendicular to *c*. The height of the propagating layer, the growth step, is one-half the c-axis length, meaning that



$t = 0$ $t = 235$ s $t = 470$ s

Crystal growth surface of beef liver catalase

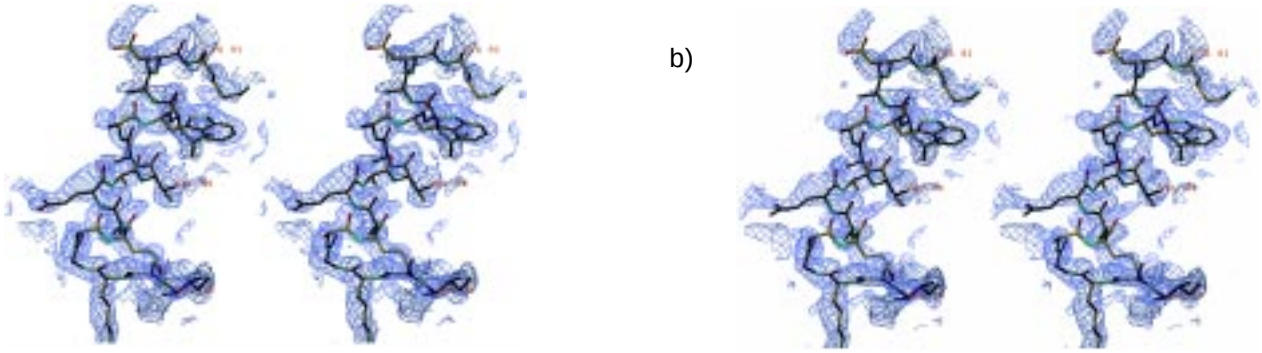
the growth step corresponds to one-half a unit cell, in this case two of the four asymmetric units. Islands of new half-unit-cell layers nucleate and propagate on the top of other layers, but the new layers have the opposite hand of the layer on which they grow. This can be seen in the figure above. Most of the island layers show a straight side and a curved side, but the sides alternate left and right between successive layers. These observations and others are discussed in the light of the crystal structure of the orthorhombic form.

One final note. A comparison of the molecular structures of catalase in trigonal and orthorhombic crystals shows that, while lattice interactions may have a profound effect on how crystals develop, they have little influence on the details of the structure of the constituent molecules.

Howard Einspahr
Bristol-Myers Squibb Pharm. Res. Inst., Princeton, NJ, USA

Two-Wavelength MAD Phasing: In Search of the Optimal Choice of Wavelength

a) b)



(a) Detail of the 2.1 Å MAD map of cytochrome *c*553 calculated with phases from the three-wavelength data set, showing an α-helix and the refined model. (b) As (a), calculated with phases from a two-wavelength data set.

Gonzalez *et al*. [*Acta Cryst.* D55 (1999), 1449-1458] reported in their recent article that interpretable electron-density maps, similar in quality to those calculated with data collected at three wavelengths, could be obtained using only two wavelengths if the wavelengths were chosen so as to give a large contrast in the dispersive component of the scattering factor. Four different crystals, which contain iron, gold, iridium, or selenium atoms, were used in their study.

The multiwavelength anomalous dispersion (MAD) method exploits the structure-factor variation with wavelengths around the absorption edges of heavy atoms within the protein crystals. The variation consists of the real part (or the dispersive component, f') and the imaginary part (or the anomalous component, f''). The importance of using wavelengths that can provide the largest f' was explained as follows: "Firstly, the refinement of the anomalous scatterer positions and occupancies is highly dependent on the dispersive differences measured from centric reflections. Secondly, a MAD data collection is usually performed in a way which partially cancels out systematic errors in the structure factors at different wavelengths, leading to dispersive differences which are less affected by errors in the data."

Two approaches have been used in calculating phase information from a MAD experiment. One approach uses an analytical method to solve the phase problem and calls for three or more wavelengths to optimize the results. The other approach treats MAD as a traditional isomorphous replacement phasing. The importance of selecting a large difference in the real part of the scattering factor in the two-wavelength experiment is interesting, as it resembles what is known from the single isomorphous replacement and anomalous scattering (SIRAS) experiment, i.e., phasing power increases with increased differences in the real part of the structure factors, which is achievable by the incorporation of heavier heavy atoms.

Most structures determined by the MAD method thus far were obtained from data collected at three or more wavelengths. Doing the MAD experiment using fewer data sets will reduce crystal exposure to X-rays and is a good option for structure determination using a high-flux synchrotron source or as an on-beamline map calculation whereby a two-wavelength map is calculated to evaluate the need, on the fly, for collecting data at more wavelengths. More interesting still, is the one-wavelength approach for on-the-fly map calculation using data from the very first wavelength, where radiation damage is the least. Using a numerical method for resolving phase ambiguity, we have recently determined the structure of an Fe-containing protein (86 kDa per asymmetric unit) using single-wavelength iron anomalous data collected in-house (P12.02.023 IUCr 99 program abstracts). For single-wavelength anomalous scattering data, collection at the absorption edge is preferable. However, the use of other wavelengths, in-house or at synchrotron, is an option provided that the measurements are accurately made.

Bi-Cheng Wang
U. of Georgia, Athens, GA, USA

Was the SDPD Round Robin Drug Biased?

The preliminary conclusions of the first Structure Determination by Powder Diffractometry Round Robin (SDPDRR) were given at ECM-18,Prague, Aug. 1998. The Web site had 800 visitors and 70 data downloads were counted, 31 participants were explicit about the software they used. Only four final participants sent questionnaires of which none determined the inorganic compound structure $[Co(NH_3)_5CO_3]NO_3 \cdot H_2O$, and only two produced the pharmaceutical compound structure $C_{22}H_{24}N_2O_8 \cdot HC1$ (tetracycline hydrochloride). One success was due to the ability of DRUID software to locate a molecule inside a cell by a "Global Optimization Method". The second success made use of the good old Patterson approach, but some additional materials, not provided by the Round Robin organizers, are suspected to have played an important role. Namely five cigarettes and two cups of coffee, as confessed by the participant, who solved the structure in 3 (very probably intense) hours. The conclusion of this Round Robin is that SDPD is not yet routine. Solving structures "on demand" by powder diffractometry requires not only good software but also some user skills. This is why crystallography is still so exciting. We should not forget the contribution of the human brain and its stimulation by the quasi drugs like caffeine and nicotine. Both structures were also solved by the organizers, with the help of caffeine. Jokes aside, one reason for so few successes could be the lack of availability of some recent packages in the public domain, particularly software allowing the location of molecular fragments in cells.

Detailed information is available at http://fluo.univ-lemans.fr:8001/SDPDRR/.

Armel Le Bail and Lachlan Cranswick

Glasgow Epilogue

An International Union?

It is the fate of most Congresses to be remembered for something difficult or troubling - like the heat in Bordeaux - as well as for all that is excellent. In the case of an otherwise happily memorable Congress in Glasgow, the one cloud of abiding regret seems likely to hang over the decision of the General Assembly to accept the invitation from Florence rather than Nagoya to host the Congress in 2005. In a week marked by a much-publicised eclipse of the sun, here was an eclipse of sweet reason.

The Congress last went to Japan in 1972 - in fact, the *only* time it has been to Japan so far in the Union's 50-year plus history. An invitation to hold the Congress there in 2002 was presented at Seattle, but the choice went to Jerusalem. This time the renewed Japanese invitation for 2005 was in competition with a first-time bid from Florence. It would anyway seem obvious in an international body that a sequence of three successive Congresses in the broadly European area could not be countenanced as long as all the rest of the world is not gripped by plague, flooded, at war, or otherwise unavailable. But the General Assembly decided to the contrary.

Possible 'reasons' for this that have emerged appear mostly to reflect exaggerated concerns about costs and local arrangements. In fact, there was nothing about the Nagoya bid that lay outside the normal range of pluses and minuses in Congress venues at all, let alone by enough to justify a supposedly international scientific body acting in such a blatantly uninternational way. Now the cost of travel to far away venues will prevent another cohort of young scientists from Japan and neighbouring Asian countries from ever attending a Congress in substantial numbers. European young scientists who might have expected to 'see the world' through two or three Congresses will not do so. And a nation that is one of the great powerhouses of modern crystallography, with a very large community, and an extraordinary range of facilities to show us, has been gratuitously rebuffed.

Maybe some of those who voted for this outcome might now regret it. It is anyway beyond doubt that considerable damage has been done to the internationality of the Union, and it behoves all who are in any position to help repair this damage to do so. And surely the Executive Committee and the General Assembly will want to consider how better to order these things in future.

None of this is in any way a criticism of the group responsible for the bid from Florence. They were fully entitled to issue their invitation, made an excellent job of it (as did the Japanese of theirs), and would no doubt have been perfectly happy to host in 2008. They now deserve the completely unqualified support of us all. But that needs to be coupled with an open acknowledgement that a very significant wrong has been done - not in choosing Florence, but in rejecting Nagoya - plus a commitment to make amends and, above all, to restore faith that the 'I' of 'IUCr' means what it says. These thoughts are offered in that spirit.

Richard Nelmes

ERICE 1999

Crystal Engineering: From Molecules and Crystals to Materials

The first Advanced Study Institute offering a coherent approach to crystal engineering as an integrated interdisciplinary area of research was directed by D. Braga (U, di Bologna, Italy) and A.G. Orpen (U. of Bristol, UK). A major challenge of the School was having teachers of organic, inorganic, organometallic, theoretical, materials chemistry and biochemistry stimulate productive interactions among experts in modeling, theoretical calculations, crystal synthesis, product design and structural characterization and manipulation of physical properties. The 500 page proceedings will provide a state-of-the-art description of the field and offer new ideas to young scientists interested in multidisciplinary fields. The lectures provoked considerable discussion, with particular interest expressed in the properties of molecular materials and non-covalent bonding. Short talks were presented by students and senior attendees and the majority of attendees presented posters. Computer tutorials on the Cambridge Structural Database, run by CCDC staff were presented at two levels of complexity depending on previous experience. Round-table discussions on (i) growing crystals and (ii) crystal engineering in industry provoked extensive debate and participation by both teachers and students.

L. Scaccianoce (Cambridge) and C. Zybill (Jena) were awarded the 1999 Erice Vaciago Prize for the most dynamical "students" in the lecture hall. The School was attended by 124 participants from 29 Nations.

Dario Braga, Course Director

Erice School of Data Mining

Crystallography was among the first disciplines to recognize the importance of computer storage of data. Databases established in the early 70's provide an opportunity to mine the wealth of knowledge they contain. The purpose of this Erice School was to provide an overview of the methodologies currently used for data mining in crystallography and outline the advances needed for a more effective and efficient exploitation of databases.

The first part of the School, devoted to methodologies and tools, provided a survey of data acquisition and validation and knowledge representation techniques and an introduction to the many paradigms of machine learning. This was followed by a journey through the various stages of data mining, from prospecting to sampling, knowledge extraction and refinement. A plethora of choices exist to extract knowledge from the databases, from visual and statistical techniques to artificial intelligence. No single approach will perform well on every problem and combining results obtained using different approaches can increase the usefulness of the data mining exercise.

The second part of the School focused on applications of data mining to structure classification and prediction, structure-activity relationships, materials design and biotechnology. Superb examples of these applications were presented in supramolecular chemistry, genomics, inter-molecular interactions and drug design.

Because data mining starts with deposits, it is necessary to provide incentives to the scientific community to deposit their data. Good results can only be obtained from good data, though, pointing to the importance of validating the data. While several methodologies have already proven useful for mining crystallographic databases, significant progress will require adopting a common language, common standards and establishing test datasets so as to put in place a more rigorous process for assessing the performance of the various tools. As databases continue to grow and initiatives such as genomics and proteomics progress, mining the databases becomes both a necessity and an opportunity.

In bringing together crystallographers and computer scientists in the beautiful surroundings of Erice, the School was described as a "first" or "blind date". The clear wish, expressed by the majority of the participants, for further interactions speaks well of the commitment of the two communities to join forces in extracting the rich scientific knowledge embedded in crystallographic databases.

Suzanne Fortier, Course co-director

La Notte d'Argento

The International School of Crystallography at Erice marked its 25th anniversary in grand style with a series of events called "La Notte d'Argento". A mixture of fantasy, humour and fun, devised by S. Fortier (Course Director, 1997 and 1999) and P. Spadon (Secretary of the School).

The 200 participants of the Crystal Engineering and Data Mining courses assembled in the S. Rocco Court displaying "argento" ornaments (long dresses, bow ties, scarves and silver beards). Accompanied by a local brass marching band, they walked through the millenarian streets of Erice, cheered by the local residents who recorded the procession on film. They were greeted in the S. Francesco court with sparkling wine and Italian folksongs. Attempts to toast and roast Lodovico by S. Fortier, J. Howard, P. Beurskens, L. Nassimbeni and H. Schenk (participants in the 1974 inaugural crystallographic course) were cut short; due to "religious" attention to punctuality in Erice, guests must not be late for dinner and face cold pasta. All participants were seated at tables for dinner, something that had not happened within the S. Francesco since the Pope's visit. A Sicilian folk group engaged the crowd in song and dance that led to dancing through the night in the court of S. Francesco.

Suzanne and Paola, all of Paola's tireless helpers, and the Goddesses of Erice (for providing mild temperature and plenty of silver stars), are to be thanked for this unforgettable night.

Lodovico Riva di Sanseverino

Macromolecular Course

A lab course on Rapid Data Collection and Structure Solving in Macromolecular Crystallography at Brookhaven National Lab in April, 1999 attracted forty-seven students including six senior scientists. A summary of the course can be found at the web site http://www.x12c.nsls.bnl.gov/rr_course/.

Two days were devoted to lectures on fundamentals and practical details of use of software and specimen handling. Lectures: •Diffraction Geometry for the Rotation Method (R. Sweet) •Strategy in data collection (Z. Dauter)•Data reduction with d*Trek (J. Pflugrath), the HKL suite (Z. Otwinowski and W. Minor) and, the DPS/Mosflm Package (C. Nielsen) •Beamline software: Optix, MARMAD (J. Skinner) and ADSC and X12-B controls (Malcolm Capel) •Frozen specimen preparation (E. Garman) •Special properties of SR: polarization, bandwidth, collimation (L. Berman) •CCD-based x-ray detectors (M. Capel) •Structure solving with MAD (C. Ogata), SOLVE (L.-W. Hung), and CNS (J. Jiang).

On the evening of the second day data collection began. Half of the students brought specimens. Some in liquid nitrogen, others in delicate crystal-growing apparatus.

Six NSLS dipole beamlines were dedicated to use by the students in the course. Nearly all of the projects accomplished useful data collectionand three teams produced useful electron density maps

During the two days of data collection there were continuing tutorials in use of the software and crystal freezing. C. Weeks of the Hauptman/Woodward Inst. demonstrated Shake-and-Bake and solved a heavy-atom problem with a student who had brought otherwise uninterpretable data and S. Parkin of Duke helped E. Garman in the crystal-freezing lab.

This course was sponsored by a grant from the National Institute of Health Div. of Research Resources to the Brookhaven Biology Dept and National Synchrotron Light Source, and in part by support from the Dept of Energy Offices of Biological and Environmental Research. Some financial assistance came from Brookhaven Science Associates and Hampton Research Corp. of Laguna Niguel, California. It was organized by R.M. Sweet, M. Capel, L. Berman, and A. Emrick.

Robert Sweet

Attendees at the Macromolecular Crystallography Course Brookhaven National Lab.

Molecular Modelling

A meeting on Molecular Modelling held at St.Batholomews's Hospital, Smithfield, London in Dec., 1998 was organized by the Industrial Physical Chemistry Group within the Industrial Affairs Div. of the Royal Society of Chemistry.

N. Quirke (Imperial College) explained that although reality is complex we have to make simplifying assumptions to make any progress in the field. People are now attempting the simulations of surface wetting, including the addition of particulates to polymers during production, where it is essential for wetting to take place.

D. Tildesley (Unilever) discussed the presence of small crystal shapes in shampoos. Some crystal shapes make the shampoo gleam more than others, which is apparently a great selling point with their customers. (Personally, I keep my eyes shut when shampooing my hair so I have not observed this phenomenon.)

R. Catlow (Royal Inst.) spoke on simulations of large scale properties such as elasticity or diffusion through structures. They are modelling zeolites for use as catalysts and looking at how the organic molecules 'dock' into the holes in the structure.

K. Gibbons (North Carolina State U.), discussed phase equilibria and confined flow, such as that through oil pipelines and at a much smaller scale through porous glasses used in chromatography.

I. Gould (Imperial College) is also working on the modelling of photosynthesis in order to produce a better type of solar cell which can use many different wavelengths of light as plants do. D. Nicolaides (MSI) talked about modelling lubricant flow round complex shapes.

Kate Crennell

Optoelectronic Materials

The "II Workshop on Optoelectronic Materials and Their Applications (including Solar Cells)", held Nov., 1998 at the U. of Havana, Cuba was attended by 35 participants from Cuba and 37 from laboratories and Universities of Mexico, Colombia, Brazil, France, Venezuela, Spain, USA and Italy. The program consisted of 14 Invited lectures and 78 contributed papers grouped in three poster sessions: I. Fundamental Properties of Optoelectronic Materials; II. Growth and Characterization of Optoelectronic Materials; III. Optoelectronic Devices and Solar Cells.

The meeting was co-sponsored by: U. of Havana, Institute of Materials and Reagents, Cuba, Int'l Union of Pure and Applied Physics, Int'l Center for Theoretical Physics, Trieste, Italy, Int'l Union of Crystallography, Latin American Center of Physics, Brazil, Dept of Physics, Northern Catholic U., Chile, Electron Devices Society.

The students supported with the funds of the International Union of Crystallography were: L. M. Hernández, M. Garcia Rocha, M. Becerri, G. Casado, R. Huerta (CINVESTAV, Mexico), and J.C. Gonzalez (Federal U. of Minas Gerais, Brazil).

The next workshop will be held in Mexico in 2000.

Maria Sanchez, Chairperson
Optoelectronics 98

Deep in the Heart of Europe

A group of 41 researchers from nine laboratories in central Europe gathered in Thuringia, Germany in Oct. 1998 for the first "Heart of Europe meeting on Bio-Crystallography" organized by M.S. Weiss and R. Hilgenfeld from the IMB and sponsored by MarResearch. The meeting gathered members of all bio-crystallography groups in the area and gave students the opportunity to present their work in an informal atmosphere. Group leaders gave an overview of the ongoing activities in the respective laboratories. The topics of the 30 presentations by students and post-docs (see http://www.imb-jena.de/www_sbx/east/east.html) ranged from crystallization and structure analyses to modeling and drug design. The meeting showed that there is lots of high-profile activity in the bio-crystallography field in the heart of Europe. .

Participants at the 1998 Heart of Europe meeting on Bio-Crystallography.

The second Heart of Europe Meeting on Bio-Crystallography", organized by Y. Muller and U. Heinemann from the MDC in Berlin, will take place Sept. 30 - Oct. 1, 1999. More information can be found at http://www.mdc-berlin.de/~crystal/heart/hec.html.

M. S. Weiss

In Situ X-Ray Analysis and Smart Materials

The 56th Pittsburgh Diffraction Conference, Nov., 1998, featured symposia on *In-Situ X-Ray Analysis* chaired by R. Snyder (OSU) and on *Smart Materials* chaired by R. Newnham. Leading off the first symposium, C. Hubbard (Oak Ridge Metals and Ceramics Div.) discussed the opportunities available for carrying out *in-situ* studies of catalytic, structural, and electronic materials kept under conditions of extreme temperature and pressure and controlled atmosphere. S. Misture (NYS College of Ceramics at Alfred U.) talked about his recent studies of Electrostrictive materials, solids which expand and contract in proportion to the square of the applied field - obviously of great practical importance. M. Rodriguez (Sandia National Labs) discussed the chemistry and development of Lithium ion batteries. J. Kaduk (Amoco) discussed localizing the cations in Zeolite Y using multi-wavelength powder data. [*Allen Hunter*]

Smart materials have the capability to both sense and respond with some useful action to changes in the physical and/or chemical conditions of their surroundings. The materials used in smart devices are highly responsive because of some inherent, persistent "disequilibrium" related to their crystallographic state; they are, in a sense, "quivering inside" in anticipation of a state change initiated by relatively subtle changes in their physical and/or chemical environment.

Smart materials such as piezoelectric lead-zirconate titanate [$Pb(Zr,Ti)O_3$] and the shape-memory alloy Nitinol [NiTi] possessing active domain walls, and two phase transformations which also allow for the ability to further "tune" a smart response of the materials. They typically possess a structural or morphotropic phase boundary [MPB], separating two phases of distinctly different symmetry. Compositions from these solid solutions remaining active and responsive over a wide range of temperatures.

The relaxor ferroelectric materials are a special class of ferroelectrics. They exhibit a more diffuse temperature dependence of their dielectric properties as they undergo the paraelectric - ferroelectric phase transition over a range of temperatures as opposed to the relatively sharp transition that is manifested for the "normal" ferroelectrics. Materials of this type tend to have exceptionally high dielectric, electromechanical, and electrooptic properties in the vicinity of this phase transition. R. Guo (Penn State) presented the crystal structure analysis and the identification of polarization mechanisms in relaxor ferroelectric tungsten-bronze materials. This family of materials is well-suited for smart applications due to their ferroelectric nature and, the presence of both a paraelectric - ferroelectric phase transition and a morphotropic phase boundary [MPB]. T. Egami (U of Penn) uses pulsed neutron

atomic pair-density function (PDF) analysis to probe the local ferroelectric structure of oxides. The results indicate that on a local scale the atomic structure of these materials is highly aperiodic, in contrast to the information typically obtained by standard crystallographic diffraction.

Q. Zhang (Penn State) discussed the first discovered relaxor ferroelectric polymer. The exceptionally high electrostrictive strains produced in these materials have been attributed to their relaxor nature, a significant lattice strain difference between polar and nonpolar regions, and the polymer's inherent capacity to accommodate larger strains without experiencing mechanical failure. S. Pilgrim (Alfred U.) spoke about the development of electroactive smart materials for control systems of communications satellites and interplanetary probes. Relaxor electrostrictive materials with transition temperatures within the range of 30 - 100 K are desirable for these purposes.

W. Soffa (U. of Pittsburgh) addressed the relationship between microstructure, defect-structure and properties of ferromagnetic alloys which are responsive to changes in magnetic field. The identification of the effects on domain structure and wall mobility have become key elements in the development of magnetic smart materials. J. Levy (U of Pittsburgh) spoke on high-resolution optical techniques for real-time imaging of domain wall movement in activated ferroelectric thin films. P. Phulé (U of Pittsburgh) described magnetorheological (MR) smart fluids that undergo a rapid and significant increase in viscosity with the application of an external magnetic field. Even though this material is referred to as a "fluid," it assumes a periodic structure that can be probed by X-ray diffraction. With the removal of the magnetic field, the material reverts back to its fluid form very much resembling ordinary paint in terms of its viscosity and physical appearance. [*Jayne Giniewicz*]

From the ACA Newsletter, Winter 1998

XTOP98

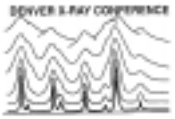
The 4th biennial conference on High Resolution Diffraction and Topography was held at the U. of Durham, UK in Sept., 1998. There were 135 delegates, 176 papers, and three "Poster Highlights" sessions in which authors were given two minutes in which to summarize results.

P. Cloetens reviewed dramatic developments in phase contrast imaging stimulated by the extraordinary phase coherence achieved with the ID19 X-ray topography beamline at the ESRF. J. Gastaldi showed how the combination of phase and diffraction imaging has thrown new light on the growth mechanisms of quasi-crystals, whose 5-fold symmetry remains of interest. A. Snigirev discussed focusing optics and X-ray microfluorescence imaging on the micrometer scale. Similarly impressive were R. Deslattes experiments to define Avogadro's number, C. Noyan's microdiffraction measurements of strains in aluminium silicon integrated circuit devices, H. Metzger's revelation of the power of grazing incidence diffraction techniques to probe the in-plane lattice parameter of quantum dot and wire structures, and C. Lucas' description of *in-situ* studies of surface reactions.

The proceedings will be published in the *Journal of Physics D*.

Brian Tanner, Conference Chairman
From the BCA Newsletter, Dec. 1998

1998 Denver X-Ray Conference



In 1951, the U. of Denver held a one-day symposium on the use of X-rays and their importance in modern research. The Denver X-Ray Conference has grown to provide a leading forum for scientists working in the field of X-ray materials analysis. The 47th conference, held in Colorado Springs, CO, Aug., 1998, was organized by a committee of eleven and run by ICDD. The conference hosted 389 registered attendees and 275 exhibitors who represented 39 companies. The program and abstract book ran to over 250 pages.

The technical program offered two days of tutorial workshops, followed by three days of invited, contributed and poster presentations on a variety of topics covering both X-ray Fluorescence (XRF) and X-ray Diffraction (XRD) techniques.

The 1998 Birks Award was presented to Horst Ebel of Technische U. Wien, Austria, recognizing his excellence in the field of X-ray fluorescence spectrometry. Herb Göbel of Siemens AG, Germany, received the J.D. Hanawalt Award for his important recent contribution to the field of X-ray powder diffraction and presented a lecture "High Temperature Studies with Oven Cameras".

Sessions covered X-ray Optics; XRF Detection Limits - How Low Can We Go?; Synchrotron Applications of Powder Diffraction; X-ray Absorption Spectroscopy; Recent Developments in Instrumentation and Detectors; and XRD & XRF; Data Treatment; Thin Films: Orientation, Stress, Thickness; Innovative Rietveld Analysis; Quantitative Phase Analysis; and Materials Process Characterization.

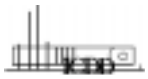
For more details and future programs visit the Denver Conference website: www.dxcicdd.com.

The proceedings of the *Denver X-Ray Conference, Advances in X-ray Analysis*, Volume 42, will be produced on a CD-ROM by ICDD; the hard copy will be published by Plenum.

Dave Taylor
From the BCA Newsletter, Dec. 1998

X-Ray Diffractometer Needed

Donation of a powder X-ray diffractometer, 220V, 50Hz, in operating condition, to Prof. Galiba Sijaric, Fac. of Science and Mathematics, U. of Sarajevo, Bosnia and Herzegovina (E-mail: sijaric@newton) would be greatly appreciated.



ICDD Scholarships

2000 Awards

To encourage promising graduate students to pursue crystallographically oriented research, the Int'l Centre for Diffraction Data (ICDD) has established a Crystallography Scholarship Fund. The year 2000 Scholarship Award has been increased to $2,250. The deadline for applications sent by FAX is Oct. 29, 1999, hard copy deadline is Dec. 1, 1999. E-mail applications are not acceptable. More information is available at http://www.icdd.com/resources/scholar.htm.

1999 Scholarships

The ICDD Crystallography Scholarship Committee has selected five winners for the 1999 Scholarship program. They are: B. DeLaBarre (McMaster U., Canada), S.P. Farrell (U. of West. Ontario, Canada), C. Lind (Georgia Inst. of Tech., USA) O. Navon (Ben-Gurion U. of the Negev, Israel) K.S. Weil, Carnegie Mellon U., USA). B. DeLaBarre's studies focus on Determining the Phases for a Difficult Protein Structure. S. Farrell's research involves Sulphur K- and L-Edge XANES of 3d Transition Metal Sulphides and Silicate and Germanate Glasses. The exploration of New Negative Thermal Expansion Materials Related to Cubic ZrW_2O_8, will be conducted by C. Lind. O. Navonís thesis research concerns Polymorphism and the Influence of Crystal Forces on Molecular Conformation. K.S. Weil will continue his Investigation of the Formation, Structure, and Magnetic Behavior of Compounds in the Nickel-Molybdenum-Nitride System.

Dorothy Hodgkin Prize 2000

Nominations are invited for the fourth award of this prize, due to be presented at the BCA Annual Conference in April 2000.

The Dorothy Hodgkin prize of the BCA was instituted on the occasion of her 80th birthday in recognition of her great contributions to science in general and to crystallography in particular. Nominations for the 2000 prize are welcomed from any part of the crystallographic community and should be received by the President of the BCA, before Sept. 30, 1999.

Information is available at: http://gordon.cryst.bbk.ac.uk/BCA/admin/PRZ.html.

Catalyzing Career Transitions to Computational Molecular Biology

The Alfred P. Sloan Foundation and the U.S. Dept of Energy (Office of Health and Environmental Research) announce the fifth round of a jointly-sponsored postdoctoral research awards program for scientists interested in computational molecular biology.

The purpose of these fellowships is to catalyze career transitions into computational molecular biology from physics,

mathematics, computer science, chemistry, engineering and related fields. The focus is upon computational molecular biology related to data and information from studies of human and other genomes. Computational molecular biology is taken broadly to include the application of mathematics (continuous and discrete), statistics, probability, and computer science to fundamental problems of molecular biology.

Awards will support up to two years of research work in an appropriate molecular biology dept or lab in the US or Canada selected by the applicant. Applicants must be citizens or legal permanent residents of the US.

The application deadline is Feb. 1, 2000. Further details are available at http://www.sloan.org.

Weinberg Wins Wood Award

The winner of the 1999 Elizabeth Wood Science Writing Award is Robert A. Weinberg, the discoverer of the first human oncogene and winner of the 1997 National Medal of Science. *Racing to the Beginning of the Road* is the fascinating personal account of Dr. Weinberg's research career. He details the uncertainty, setbacks, discoveries, and achievements in cancer research for the past 30 years. I recommend the book for young people considering a career in science because it conveys the challenge and excitement of experimental science. ACA members will enjoy his description of the personalities and controversies which have been an integral part of the stories.

Virginia Pett, from ACA Newsletter, Spring 1999

Industrial Group Award

David Rendle was presented with the 1999 Industrial Group Award of the British Crystallographic Assn. The award recognized his contributions to the application of crystallography in forensic science.

Rendle studied at Loughborough U. of Technology, the Universities of Waterloo and Guelph, and the U. of British Columbia. He joined the Metropolitan Police Forensic Science Lab in 1975. He published papers covering sample preparation, paint pigment analysis, drugs and metabolite identification, the use of soft X-rays for detecting forgeries, re-sealed envelopes and even serial numbers filed off engine blocks. All this work has been carried out to the exacting standards needed for a Court of Law.

An active member of ICDD, he has championed the cause of organic phases in the Powder Diffraction File and currently chairs the Organic Materials sub-committee.

Steve Norval
BCA Crystallography News, June 1999

Awards to Crystallographers

•The American Assn for Cancer Research presented John Kuriyan, Howard Hughes Medical Inst. investigator, with the Cornelius P. Rhoads Memorial Award for his X-ray crystallographic studies of structure and interactions of critical genes and control factors involved in transcription.

•The Biophysical Society announced the Society Award winners for 2000. Helen Berman received the Distinguished Service Award for service in the field of biophysics and Carolyn Cohen received the Elisabeth Roberts Cole Award for outstanding achievement in biophysics.

•R. Bott, Genencor Int'l was named co-recipient of the 1999 American Chemical Society Award in Analytical Chemistry.

•Suzanne Fortier (Professor and Vice-Principal of Research at Queen's U. in Kingston, Ontario) is the new Vice-President of the NSERC (Nat'l Science and Engineering Council). She is currently Chair of the Ontario Council on University Research, and a member of the boards of two Ontario Centres of Excellence. In 1997, she received the Clara Benson Award for distinguished contribution to chemistry by a woman, and the Entrepreneurship Award (with J. Glasgow and E. Steeg), a Communications and Information Technology Ontario Innovation Award.

CrystEngComm On-Line

Crystal engineering excompasses rational crystal syntheses and design and the evaluation of the physical and chemical properties of the resulting crystalline materials. The Royal Soc. of Chemistry has announced the start of a new electronic journal on crystal enginering: CrystEngComm. The Editorial Board is formed by D. Braga (Scientific Editor), G.R. Desiraju, J. Miller, A.G. Orpen, S. Price and J. Humphrey (RSC Managing Editor). Publication of the first issue is scheduled for Oct. 1999. Submissions are invited.

CrystEngComm is a forum for the electronic publication of significant original research in all branches of crystal engineering. CrystEngComm aims to develop synergetic interactions between those involved in the design, synthesis, characterization, modeling, and theoretical evaluations, of building blocks and new materials and to further the exploitation of their physical properties. CrystEngComm targets a broad interdisciplinary research community; thus, submissions to CrystEngComm must have wide general appeal or be of exceptional interest in a specialized area. Further instructions for submission are available at http://www.rsc.org/CrystEngComm. Direct information may also be obtained from D. Braga, U. of Bologna (dbraga@ciam.unibo.it or CrystEngComm@rsc.org).

Dario Braga

Chemical Crystallography Goes On-line

Robin D. Rogers editor of *J. Chem. Crystallography* announced that the journal will be online starting in 1999. Newly appointed board members are C. Aakeröy, G. Desiraju, D. Braga, and Z. Schpector. The journals publisher, Plenum, has been purchased by Kluwer.

Cuban Chemical Congress

The Third Int'l Cuban Chemical Congress, in Dec. 1998, covered all areas of chemistry and was especially rich in environmental chemistry and chemical education. Although handicapped by restricted communication with the United States and limited availability of some advanced technologies Cuban scientists continue to make significant contributions to science. Herb Hauptman who presented one of the plenary lectures at the Congress expressed grave concern about the lack of diffraction equipment in Cuba. A C & E News reporter noted that Hauptman "invented" X-ray crystallographic equipment along with Nobel co-recipient chemist Jerome Karle. Herb and Jerry are thinking of inventing the light bulb next.

A New Type of Hydrogen Bond

The π electrons of an aromatic ring can sometimes act as an H bond acceptor to form an X-H…π hydrogen bond. Surprisingly in a structure containing the arrangement acceptor X-H…H-Y the H…H distance, typically 1.9Å, is much shorter than the normal H…H contact of 2.5 Å [R.C. Stevens, et al, Chem. Soc. Dalton Trans, 1990 1429, L.S. Van der Shiys et al, JACS 112, 4831 (1990)]. This Y-HT attractive interaction between two hydrogens has come to be called the "dihydrogen bond". Y is always an electropositive atom such as boron or a transition metal. A neutron-diffraction structure of H_3BNH_3 (Koetzle, unpublished) unambiguously show the presence of short H…H contacts (2.02 to 2.23 Å), but the most surprising aspect of this work was the demonstration that boron and nitrogen had been misassigned in the previous X-ray work.

Robert Crabtree in Science Vol 282 Dec 98

Look Ma, No Crystals

David Sayre and co-workers have created the first diffraction images from noncrystalline samples, a feat that could revolutionize the imaging of a vast array of materials that cannot be crystallized, providing ultrahigh-resolution images of everything from cells to individual protein molecules. The first images are of an array of tiny gold dots with a resolution of 75 nanometers. That doesn't match the resolution available from X-ray diffraction of crystalline samples, but it is better than the best optical microscopes. Generating enough diffraction data from a single molecule will require new X-ray sources billions of times brighter than today's.

R. F. Service, Science, Vol 285, July 1999.

CLRC

The December 1998 issue of the BCA Newsletter contained a nine page CLRC report on users meetings and instrument improvements from the Daresbury and Rutherford laboratories combined with information on protein and materials application, new stations, and new detectors and the ever increasing demand for access to the facilities.

Measuring stress with neutrons. The measurement of stress using neutron diffraction is a rapidly growing field, of great relevance both to the academic materials science world and to the industrial world of structural engineering. Recent efforts to introduce an international standard for neutron stress measurement, coupled with European Union funded ventures to bring the technique to a broader range of industries are stimulating an increasing interest in the technique.

Increasing demand and international standards. Industrial demand has led to two European funded networks with members from industry, academia and neutron facilities. RESTAND, a network run by the JRC in the Netherlands aims to establish best practices for neutron measurements. TRAINSS, a network run by ISIS in the UK, aims to introduce industries to the technique and train them in measurement practice and interpretation.

The VAMAS TWA20 initiative, headed by Imperial College, London, is made up mostly of academics and representatives from facilities around the world; it is working to define an international standard for stress measurement using neutrons. The project will involve four different round robin samples which will be measured at each neutron facility. Each is typical of a problem found in real measurements: high strain gradients, multiple phases, through surface strain measurements, and large compositional variations.

A training network has been proposed to help cope with the increasing demand from academic users. This will allow novice users to accompany more experienced ones on experiments at neutron facilities where they will learn by example, helping with the experiments and discussing the results and their interpretation. Help with proposal writing will also be given.

Anyone interested in using neutrons for stress measurement, or any other applied applications, is encouraged to contact M. Daymond, email: mark.daymond@rl.ac.uk. Tel: 44 0 1235 445414.

From BCA Newsletter, December 1998

DARTS - Synchroton Radiation Service

The DARTS data collection service, EPSRC-funded, is to provide access to SR data, using a wide range of techniques (including powder diffraction, reflectivity, small and wide angle scattering and X-ray absorption spectroscopy), to academics who are inexperienced in its use and applications. The service is to be extended to incorporate single crystal diffraction using the microcrystal facility on station 9.8 of the SRS.

Academic access to the service is available to any researcher eligible to apply for research grants from EPSRC, http://www.dl.ac.uk/SRS/.

The CCP4 Program Suite

The Collaborative Computational Project No. 4 (CCP4) is an initiative of the UK Biotechnology and Biological Sciences Research Council for the development, maintenance and distribution of a software suite for protein crystallography. Applications include data reduction, scaling programs, Patterson search and refinement, isomorphous and molecular replacement, MAD phasing, phase improvement (density modification), structure refinement and presentation of results. The suite is ported to most UNIX systems, including LINUX, as well as VMS. The Suite included 130 programs, and was used at around 400 sites worldwide.

A central part of the suite is a library of routines commonly used in crystallographic applications and these may be useful in non-CCP4 programs (see http://www.dl.ac.uk/CCP/CCP4/dev/templates/templates.html).

Version 3.5 will contain the following new programs:

*DYNDOM: Program to determine domains, hinge axes and hinge bending residues in proteins where two conformations are available (S. Hayward), *MTZMADMOD: Jiffy for converting between F+/F- and F/D, *FINDNCS: Find out NCS operations from heavy atom sites (G. Lu), *WATNCS: Pick waters which follow NCSs and sort out to NCS asymmetric unit (G. Lu), *TOP: An automatic structure comparison program and web server (G. Lu).

The suite is available free to non-profit institutions, subject to a completed license form being returned to the CCP4 secretary. A charge is made to commercial users who should contact the CCP4 secretary at ccp4@dl.ac.uk to make arrangements. All charges for the suite are used to fund CCP4 activities. Further details on obtaining the Suite can be found on the CCP4 web site http://www.dl.ac.uk/CCP/CCP4/main.html.

Inquiries may be sent to the staff at Daresbury Lab, (M. Winn, A. Ashton, P. Briggs and S. Bailey) email: ccp4@dl.ac.uk.

Martyn Winn, Daresbury
from BCA Newsletter, March 1999

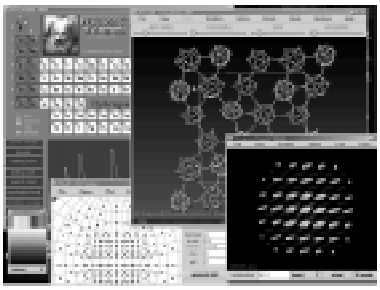
Free Software

A selection of DOS and Java computer programs covering various crystallographic aspects may be downloaded from my website (http://www.nirim.go.jp/~weber): structure display; diffraction pattern simulations (Laue, precession, powder, Kossel); stereographic projections; 3D reciprocal space visualization; point groups; wallpaper patterns; quasiperiodic tessellations; polyhedra and crystal shapes; vector visualization; periodic tables; Fourier transforms (FT); difference plot.

Steffen Weber

Editor's Note: Steffen asks you to make a contribution to UNICEF if you like his programs and continue to use them.

Academic Software



The Higher Education National Software Archive (HENSA) is on the www, the part for micro computers is at http://micros.hensa.ac.uk with sections for PCs, Macs, and Acorn. You can find versions of the popular protein display package RASMOL, a public domain ray tracing package POVray, and PGPLOT a portable graphics package written in Fortran77 (for details see http://astro.caltech.edu/~tjp/pgplot/).

The ISIS supported analysis software, GENIE, now uses PGPLOT for its graphics. (http://www.ISIS.rl.ac.uk/OpenGENIE). ORNL, the originators of ORTEP, the thermal ellipsoid drawing program, have added an interface to PGPLOT to simplify porting ORTEP across to new computers. (http://www.ornl.gov/ortep/ortep.html). D.S.Sivia has written a set of routines PGXTAL, for 3D plotting structures and density maps with PGPLOT (http://www.isis.rl.ac.uk/dataanalysis/dsplot).

from the BCA Crystallography News, Mar. 1999

The ***Commission of Powder Diffraction***, Newsletter No. 21, May 1999 contains a summary of Powder Diffraction activities in India (Editor Siba Sen-Gupta) and a description of eight programs for powder analysis. Available at http://www.iucr.org/iucr-top/comm/cpd/Newsletters/.

The delegates to the 18th Congress of the IUCr represented 37 countries. The Executive Committee that presided over three evenings of discussion and deliberation are seated in the front row in this picture (from left): Michael Hart, Hartmut Fuess, Past President Phillip Coppens, President Ted Baker, Sine Larsen, President-elect Henk Schenk, Jan Boeyens, A. Aslanov, and M. Tanaka. Among other things, the delegates reconfirmed Israel as the site of the 19th Congress in 2001, chose Florence, Italy as the site for the 20th Congress in 2005 and passed a resolution to shorten future congresses by at least one day, beginning in the year 2005.

X-ray Powder Diffractometry

The International Centre for Diffraction Data (ICDD) is pleased to announce the first in a series of three-day workshops on X-ray Powder Diffractometry, Dec. 6-8, 1999, St. Helens College, St. Helens, Merseyside . The workshop is intended to train participants in all aspects of X-ray Powder Diffractometry, including "best practices" for acquiring data and phase identification using the Powder Diffraction File. Topics will include diffractometer set-up and calibration, specimen preparation, and semi-quantitative phase analysis.

For information contact T. Maguire, ICDD, 12 Campus Blvd., Newtown Square, PA 19073-3273, USA, Fax: 610 325 9823, Clinics@icdd.com; www.icdd.com.

ACA 2000

The Annual Meeting of the American Crystallographic Assn will be held July 22-27, in St. Paul, MN USA. The Transactions Symposium will be on using crystallography to understand biological mechanisms, encompassing molecules of all sizes. Two workshops are planned for July 22; SHELX for twins and macromolecular structures; and making technical presentations. Session topics will include: hot new structures, refinement at ultra-high resolution, battery materials, advances in small-angle scattering cool structures, general interest, new science from neutron sources, protein-nucleic acid interactions, high throughput crystallization, service crystallography at synchrotrons, crystal engineering (dedicated to Peggy Etter), science at long-length scale, nuclear industry materials, problem structure determination and network glasses.

Purnell W. Choppin, President of Howard Hughes Medical Inst., will be presented with the ACA Public Service Award for 2000. A special session recognizing the activities of the HHMI in biomedical research and crystallography is being planned for Wednesday, July 26.

The abstract submission deadline is March 1, 2000, with online submission beginning in January. For more details visit www.hwi.buffalo.edu/aca/.

ECM19

The 19th European Crystallographic Meeting will be held Aug. 25-31, 2000 in Nancy France. Claude LeComte is General Chair.

Microsymposiums will include: Macromolecular Crystallography, Charge, Spin, Momentum Density, Aperiodic Crystallography, Electron Crystallography, Mineralogical Crystallography, Instrumentation And Experimental Techniques, Molecular Interactions And Recognition, Surfaces Crystallography, and Powder Diffraction. Satellite meetings include: Macromolecular Crystallography (A.D. Podjarny, Chair), Electron Density Analysis (N.K. Hansen, Chair), Crystal Growth (G. Marnier, Chair), Advances in Texture Analysis of Polycrystalline Materials (J.J. Heizmann, Chair), and Surface Crystallography (P. Mangin, Chair).

The abstract deadline is May 1, 2000. More information is available at http://www.lcm3b.u-nancy.fr/ecm19/.

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Meetings Calendar

A selection of future meetings. Extensive lists appear regularly in *J. Applied Crystallography*, the *BCA Newsletter* and the *ACA Newsletter*. Corrections and new listings are invited by the Editor.

JANUARY 2000

24 - 26 ♦ **Fourth LANSCE User Group Meeting.** Los Alamos, USA. Contact: A.L. Archuleta, LANSCE User Program Coordinator, Los Alamos Neutron Science Ctr (LANSCE), MS H831, Los Alamos, NM 87545 USA, FAX: 505-667-8830, lansce_users@lanl.gov.

FEBRUARY 2000

1–4 ♦ **21st Meeting of the Soc. of Crystallographers in Australia (SCA).** Thredbo, New South Wales. Contact: http://rsc.anu.edu.au/~welberry/crystal21/.

13-17 ♦ **The 2000 Biophyscial Soc. Meeting. New Orleans, LA USA.** Contact: http://www.biophysics.org/biophys/society/annmtg.

APRIL 2000

24-28 ♦ **Materials Research Soc. Spring Meeting.** San Francisco, CA USA. Contact: http://www.mrs.org/meetings/spring00/.

MAY 2000

20-23 ♦ **7th European Powder Diffraction Conf. (EPDIC-7).** Barcelona, Spain. Contact: http://www.icmab.es/epdic7/

25-4 ♦ **Methods in Macromolecular Crystallography.** Erice, Italy. Contact: http://www.geomin.unibo.it/orgv/erice/johnson.htm.

25-4 ♦ **Prospectives in Crystallography of Molecular Biology.** Erice, Italy. Contact: http://www.geomin.unibo.it/orgv/erice/johnson.htm.