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Henk Schenk

I am proud of our six journals, their quality and their staff. The journals belong to the highest in citation rankings in their class, give great value for money, particularly compared with commercially run journals, and, moreover, they provide easy access through the Internet. Our community sets the standards and maintains them through the Commission on Journals chaired by John Helliwell. As a not-for-profit organization, the IUCr is also able to keep the journals reasonably priced. There is even a substantially reduced rate for individual crystallographers: personal subscriptions to our journals are real bargains! In my laboratory it is a tradition that the oldest staff member is a personal subscriber and it is really great to have the most important crystallographic journals on your own desk! Therefore I am surprised that the total number of personal subscribers is not higher. Today, with web access to the brand new articles, and in due course also to all back issues, it is even more attractive to subscribe. In this *Newsletter* you will find more information or you may contact our Promotions Officer Andrea Sharpe (as@iucr.org).

As Durward Cruickshank wrote [*Acta Cryst.* (1998), A54, 687-696, or in *Crystallography Across the Sciences*, same pagination], at the end of World War II such famous crystallographers as Paul Ewald, Martin Buerger and Henry Lipson formed ideas to set up a new international journal of crystallography and other services for crystallographers. Their ideal way to organize this was through an international society or union, representing the new crystallography. And so they did. As we know today they were very right in founding the Union and starting *Acta Crystallographica*. In 1948, the first year of *Acta*, 348 pages of high quality scientific papers were published containing many highlights that are still well known. We now own six journals and in 1999 published almost 1500 high quality papers in 7700 pages.

In principle the journals are still run in the same way as in 1948, although all the processes involved (editing, refereeing, technical editing) used to be in the hands of volunteers. The editing and refereeing are still done by top scientists who volunteer to keep the standards of our journals high. The technical editing is carried out by the Chester staff and this has led to many improvements such as 'Crystallography Journals Online' and an email-alerting system, and a web-based refereeing process is being developed.

The six journals form a treasure-trove for the IUCr and give us a large responsibility to keep them alive and vibrant. So we as individuals must support our sextet and there are many ways to do this:

- submitting our best scientific work,
- convincing our library to subscribe or maintain subscriptions,
- subscribing personally to one or more of the six,
- including in all our publications any relevant citation to papers in the six,
- serving as a (fast) referee,
- suggesting improvements, etc.

My last paragraph is about something completely different. As ex-Chair of the subcommittee on the Union Calendar I know that many congresses are organized all over the world and luckily also in emerging countries. Last January I was much impressed by the meeting on 'Characterization of Nanocrystalline and Amorphous Materials', organized in Ismailia at Suez Canal University by a Committee of the Egyptian Crystallographic Society chaired by Professor Karimat El-Sayed. The programme, the organization and the meeting place were all excellent and well over 100 participants met in an international setting!

Henk Schenk  
schenk@chem.uva.nl



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, Czech Republic, France, Italy, Japan, Poland, South Africa, Switzerland, and The Netherlands 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.

If you would like to see a copy of the *IUCr Newsletter* in your college or university library, send the address to the Newsletter office so that we can add it to our mailing list.

Dear Bill,

The article about twinning (page 5 of Volume 7, No. 4) appeared in the November 1999 issue of *Acta C* (the reference is correct), but the *Acta C* cover shown is the October issue.

Michael Bolte

Dear Dr. Bolte,

The miniature cover logos are a device to highlight the fact that the articles concern papers in the various IUCr journals. For the logos we used issues of the journals available in Buffalo at press time and did not mean to imply that the covers correspond to the issues in which the articles described appeared. Due to costs associated with processing illustrations, we may use the same logos repeatedly, for example, we use an old photo of me to save money and serve my vanity.

Bill

Dear Editors,

The signature under the IUCr Congress Reports, page 10 "X-ray and Neutron Complementarity (volume 7 number 4, 1999) which I wrote is wrong.

My name is BENTE LEBECH (as stated in the Congress program) and I am a woman.

Bente Lebech

Dear Dr. Lebech,

I apologize for the error. I think it is particularly important that women in science be properly acknowledged and I greatly appreciate the fact that you were one of the minority of session chairs who submitted a report.

Bill

## Observing Electron Density

*An article by Zuo et al concerning charge density studies published in Nature (401, 21; 1999) was accompanied by comments on the significance of the work by Colin Humphreys (U. of Cambridge), past chairman of the IUCr Commission on Electron Diffraction. M.A. Spackman, J.A.K. Howard, and R. Destro wrote a letter to Nature expressing concern about Humphreys' comments. The Spackman letter, which Nature declined to publish, is printed here.*

The news and views article by Humphreys (*Nature* 401, 21; 1999) commenting on the recent charge density work of Zuo *et al.* on Cu<sub>2</sub>O was welcome in the pages of *Nature*, but one could be forgiven for gaining the impression that detailed imaging of bonding electrons in crystals is a rare feat. Fortunately, that is nowhere near the truth. Extraction of detailed electron density distributions of organic, organometallic, inorganic, ionic metallic and mineral crystalline systems from X-ray diffraction data is now a mature and highly productive field, and one of the most dynamic areas of modern X-ray crystallography. It embraces not only advances in single crystal X-ray diffraction (for example synchrotron radiation and high-speed data collection), but increasingly incorporates data from complementary methods, including powder diffraction, electron diffraction, polarized neutron diffraction, and theoretical and computational chemistry. An excellent introduction is afforded by recent monographs by Coppens (1) and Tsirelson and Ozerov, (2) and virtually all experimental work performed in the field in the years 1992 - 1997 has been conveniently summarized in two review articles. (3, 4) Humphreys statement that X-ray diffraction "is normally unable to give details about the shape of the charge distribution, in particular the shape of the bonds" is completely untrue, and he goes on to erroneously attribute this to the fact that X-ray scattering from dislocations and defects "is greater than the scattering from bonding electrons". In the overwhelming majority of modern experimental charge density studies, even those based only on X-ray diffraction; this is emphatically not the case. Such studies are now commonly performed at cryogenic temperatures, use synchrotron sources as well as more conventional laboratory X-ray sources, and CCD cameras as well as increasingly sophisticated detectors. These studies are now yielding not only the shape of the bonds, but a vast amount of chemical and physical insight based upon a three-dimensional picture of the electron distribution in the crystal. Dipole and higher moments of molecules in the crystal, electrostatic potentials, electric fields and electric field gradients at atomic nuclei, and even intermolecular interactions energies are common outcomes, and the total electron distribution is now almost routinely analyzed using Bader's quantum theory of atoms in molecules, (5) affording additional detailed insight into bonding in crystals. The work reported by Zuo *et al.* is significant, in that it represents an excellent example of the synergistic interaction between X-ray diffraction, electron and modern theoretical methods as described above. But many more studies of this calibre have been published and are currently in progress. It is disappointing to us that Humphreys appears to have been unaware of them, and hence failed to put the work in the much broader perspective that the field deserves.

(1) P. Coppens, X-ray Charge Density and Chemical Bonding, Oxford Univ Press, NY, 1997; (2) V.G. Tsirelson and R.P. Ozerov, Electron Density and Bonding in Crystals, Inst of Physics Publishing, Bristol, 1996; (3) M.A. Spackman and A.S. Brown, Charge Densities from X-ray Diffraction Data, Ann. Rep. Prog.Chem., Sect. C, Phys. Chem., 91, 175-212, 1994; (4) M.A. Spackman, Charge Densities from X-ray Diffraction Data, Ann. Rep. Prog. Chem., Sect. C, Phys. Chem., 94, 177-207, 1997; (5) R.F.W. Bader, Atoms in Molecules - Quantum Theory, Oxford Univ Press, Oxford, 1990.

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**Send us  
your  
comments**

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I am pleased to report a favorable response to a request for more information about crystallography in member countries of the IUCr. A letter was sent to representatives of national committees requesting information on crystallographic organizations, laboratories and activities in their countries. Material received from China, France, Israel, Poland, Serbia, Australia, the UK and the US appears on page 16.

Other countries covered in meeting reports include India, Moldova, Germany, and Japan. If your country is not represented, we welcome your contributions. Information on awards to and elections of crystallographers are especially welcome. Because Lithuania is not presently a member of the IUCr, Kazimierz Lukaszewicz sent the names of crystallographers in Lithuania to be added to the newsletter mailing list. If you can suggest names of crystallographers in countries not in the Union who can be added to the mailing list and invited to act as IUCr reporters, that would be greatly appreciated.

It saddens me greatly to report the recent loss to the crystallographic community of too many of its founders and leaders most recently, including Jeremy Cohen, Howard Evans, George Jeffrey, Zdzislaw Galdecki, Shizou Miyake, Don Rogers, Paul Sigler, and Jürg Waser.

This is the first issue having more than 24 pages since March 1996. Larger issues cost more to produce and distribute, but the introduction of new features and accumulation of meeting reports, honors and awards made it necessary to expand this issue.

The American Crystallographic Assn (ACA) the North Ameri-

can Regional Affiliate of the IUCr is celebrating its 50<sup>th</sup> anniversary in St. Paul, Minnesota, July 22-27, 2000. Sessions will cover all aspects of crystallography. Highlights will include the Transactions Symposium "Using Crystallography to Understand Enzyme Mechanisms", workshops on SHELX, the Cambridge Structural Database and How to Make Technical Presentations, the Buerger Award lecture of Lyle Jensen and the Warren Award lecture of Ian Robinson. The ACA will present its Public Service Award to Purnell Choppin, recently retired President of the Howard Hughes Medical Inst. at the Golden Anniversary Banquet. Efforts are under way to bring together as many of the charter members of the ACA who were present at the first meeting in Penn State in 1950 and as many of the 33 living past presidents as possible. The abstracts for the meeting are on the web at [www.hwi.buffalo.edu/ACA/ACA00/abstracts](http://www.hwi.buffalo.edu/ACA/ACA00/abstracts).

The European Crystallographic Assn, the European Regional Affiliate, will hold its 2000 meeting in Nancy, France August 25-31. The ECM meeting consistently covers all aspects of crystallography with a depth and range that is only matched by the IUCr Congress. Eleven plenary lectures and fourteen microsymbosia gathered under eleven subcategories (aperiodic systems, charge spin momentum, computing, diffraction physics, electron crystallography, extreme conditions, instrumentation, biological materials, macromolecular methods, molecular interactions, powder diffraction and mineralogy) are required to cover the field and this doesn't include eleven additional microsymbosia needed to address topics such as ferro electricity, twinning, industrial applications and surface structure and function. The abstract deadline is May 1<sup>st</sup>. For additional information see the ECM-19 home page at <http://www.lcm3b.u-nancy.fr/ecm19/>. Get thee to a crystallography meeting (they are more fun than a nunnery).

## Worth Shouting About!

The IUCr has plenty to shout about. But small scientific society publishers are traditionally shy about advertising their wares. They are more likely to rely on their long-standing reputation within the community they serve, and to plough all surplus income into journal development and good works such as student training and travel support. But at the XVIIth IUCr Congress in Seattle in 1996, it was decided that the IUCr should no longer hide its light under a bushel, and a Promotion Committee was born.

The journals have a central role in advancing, promoting and sustaining quality in crystallography, and the Promotion Committee (Chair Mike Glazer) has overseen the start of a campaign to market the IUCr journals to structural science communities in biology, chemistry, materials science and physics as well as crystallography. Increased exposure at meetings will include the sponsorship of poster prizes and distribution of literature. Making ordering easy is one of the basic premises of marketing, and online order forms, bound subscription cards and advertisements are designed to increase sales. If you wish to receive a copy of the "IUCr journals 2000" leaflet, please send requests to [as@iucr.org](mailto:as@iucr.org).

We hope the IUCr journal article reviews that appear in the *IUCr Newsletter* and our e-mail announcements will tempt you to visit the IUCr's online journals at <http://journals.iucr.org>. Please take a moment right now to experience this exciting and innovative electronic service, a powerful research tool worth shouting about!

Andrea Sharpe, IUCr Promotions Officer

## IUCr Journals; Past, Present and Future Perspectives

These rapidly changing and challenging times in scientific publication provide new opportunities for publishers, authors and readers. For the IUCr this scene is set in the context of its core activities:- (i) service to crystallography and its cognate subjects, biology, chemistry, physics and materials, (ii) service to the crystallographic community, especially young scientists around the globe.

The technical editing, management and R&D staff of the IUCr journals in Chester is made up of 18 people who work closely with the Editorial Boards of the journals, 100 academic specialists in the fields covered by the six journals. The editors comprise the Journals' Commission (JComm), which holds meetings at topical conferences, at the triennial IUCr Congresses, and at meetings of the regional affiliate societies (ACA, ECA and AsCA). Because our percentage journal 'profits' should be modest, we generate a reasonable surplus for good works by having as large a volume of activity as possible. Indeed 70% of the IUCr's cash flow involves the journals, with 80% of this being *Acta Crystallographica*, 12% *Journal of Applied Crystallography* and 8% *Journal of Synchrotron Radiation*.

The founders of the IUCr foresaw the importance of its journals and entrusted their initial development to P.P. Ewald. Today the Editorial Boards are very conscious of the stewardship



Andrea Sharpe and Henk Schenk at the IUCr Exhibit booth in Glasgow.

that they inherit. They are the most public spirited and conscientious group of people I have ever worked with, giving generously of their expertise in the service of authors and readers.

The quality of the journals is ensured by the teamwork of the Chester staff and JComm. The WWW has provided rapid and efficient communication between the IUCr staff and its Editors, streamlined peer-review procedures and permitted the development of additional author and reader services culminating in *Crystallography Journals Online*. This service includes the 50-year searchable index, a fantastic research tool. Digitization of all the 190,000 published pages going back to 1948 is in progress. As a result, preparation of CD-ROMs devoted to specific topics or works of individual authors will be feasible.

Staying at the forefront of crystallographic publishing requires not only state-of-the-art author and reader services, but also Editorial Boards of exceptional depth and breadth. In addition, the IUCr has a network of Commissions whose members provide an extra body of people who are accessible for consultation on specific matters; an example is the Commission on Crystallographic Nomenclature (Chair Sidney Abrahams). The IUCr also convenes expert working groups on particular topics; of special relevance to the journals are the Committees for Electronic Publishing (Chair Howard Flack), Crystallographic Databases (Chair Frank Allen) and Promotion (Chair Mike Glazer). The IUCr subsidizes worldwide distribution of its *Newsletter* to 15,000 readers, alerting them to journal activities with journal article highlights and special issues such as this.

In the following report the Managing Editor and the R&D Officer describe journal developments. Reports follow from the individual journal Editors who describe the trends in their scientific fields and sub-fields, and future themed issues. They also mention the new Co-editors that have joined JComm recently, and their scientific interests. We hope you find their reports useful and informative and invite your comments.

John Helliwell, Editor-in-Chief of *Acta Cryst.* and  
Chairman of the IUCr Commission on Journals

## Journal Developments

The Glasgow Congress saw the latest stage in the electronic development of IUCr journals – the launch of Crystallography Journals Online, the culmination of years of work by the editorial and research and development groups at the Chester Office.

In recent years developments at the Chester Office have been geared to ensuring the rapid, accurate and high-quality publication of the Union's journals, *Acta Crystallographica*, *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation*. Our aims have been to improve the speed of publication, increase the efficiency of review, technical editing and printing processes, and provide electronic versions of the journals.

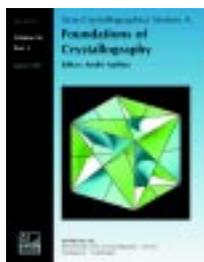
Nearly all the production work on the journals is now carried out in Chester. Manuscripts, typically submitted in CIF, Microsoft Word and TeX formats, are converted to SGML (standard generalized markup language), the publishing industry standard for electronic publishing. The SGML is then used to drive the typesetting process, as well as acting as the source for the online versions of the journals.

Pilot projects have been started to look into electronic submission and review procedures. Proofs and reprints are now routinely supplied in Adobe Acrobat PDF format, and from the start of 2000 authors have been given permission to load these electronic reprints on their personal web sites.

Crystallography Journals Online has been developed with the needs of the crystallographic community in mind. It currently provides full text versions of all of the IUCr journals in both HTML and PDF formats, and all supporting data are made available *via* the IUCr electronic archive. Other services such as e-mail alerting, tables of contents and details of forthcoming papers are available. Crystallography Journals Online currently links into the Medline and PDB databases, and it is our intention to work with other relevant bibliographic and structural databases, and primary publishers to improve linking to and from the journals.

Free access to Crystallography Journals Online has been extended until May 2000. Make sure that your library has a subscription before this date to ensure that you continue to have access to the service.

Peter Strickland, Managing Editor, and  
Brian McMahon, R&D Officer



## Acta Crystallographica Section A: Foundations of Crystallography

*Section A* of *Acta Crystallographica* is the reference journal for the "foundations of crystallography", taken in the broadest sense. It covers all experimental and theoretical studies of the properties of the arrangements of atoms, ions and molecules in condensed matter, ideal or real, and of their symmetry. The journal also deals with the theoretical and experimental aspects of the various methods used to determine these arrangements, in particular diffraction physics. Its impact factor is very high (2.146 in 1998 – the latest year for which information is available) and it ranked 3rd out of 18 crystallography journals in 1998.

*Section A* acquired a new visage in January 2000. It has adopted a contemporary format in line with the other sections. More importantly, like all the other IUCr journals, it is being produced electronically and this will bring about quite a revolution, not least in speeding up the manuscript handling process. Speed of publication is of paramount importance and the object of continuous effort, both by Co-editors and by the editorial staff in Chester, with recent marked results.

Our Editorial Board is regularly updated to keep pace with new or growing areas and topics. Electron crystallography, linear chain assemblies and crystallographic phase determination are the areas of interest of newcomer D.L. Dorset (Hauptman-Woodward MRI, Buffalo) while E.F. Weckert (U. of Karlsruhe) brings expertise in dynamical diffraction, the phase problem and structure determination. Another new face is Y. Amemiya (U. of Tokyo), who already serves on the Board of the *Journal of Synchrotron Radiation*. Prof. Amemiya specializes in X-ray physics, X-ray instrumentation and diffraction physics, and completes a team designed to uphold standards in the foundations of crystallography.

Andre Authier, Editor



## Acta Crystallographica Section B: Structural Science

In common with the other sections of *Acta*, *Section B* presents a fresh new image for Y2K – no bugs, just a much enhanced presentation of Structural Science. These upgrades are possible owing to technological advances that allow the IUCr's journals to significantly improve their position as world leaders in crystallographic information provision. The technology also underpins exciting new developments in electronic manuscript handling and the availability of published papers *via* Crystallography Journals Online. The impact of these changes is summarized in an Editorial, "*Section B* enters the electronic era", that accompanies the February 2000 issue.

The most important concern for *Section B* is the quality and breadth of its scientific content. Since 1983, its remit has been to publish original scientific research in which "structure" is the central theme. During the 1990s, this remit has extended to include high-quality Lead Articles and Topical Reviews.

*Section B* covers a broad chemical spectrum from inorganics and minerals through metallo-organics to purely organic compounds. Within that spectrum, *Section B* has continually reflected the enormous impact of crystallography in structural science. Today, current leading-edge developments include experiments at nonstandard temperatures and pressures, studies of novel materials and their physical properties, phase transitions, charge densities, intermolecular interactions, supramolecular structural organization, crystal engineering, database applications, and the burgeoning field of structure determination from powder data. The Editorial Board has been enhanced in recent months by the appointment of S. van Smaalen (U. of Bayreuth) and G. Chapuis (U. of Lausanne) to provide additional expertise in inorganic and materials structures.

Frank Allen, Editor



## Acta Crystallographica Section C: Crystal Structure Communications

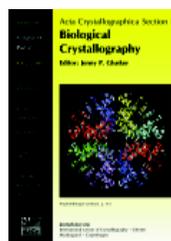
Starting with the January 2000 issue, there have been significant changes to the format of *Acta Crystallographica Section C* and all *Section C* articles, including the new category of electronic papers, are available online.

For *Section C* full-paper submissions, authors are asked to focus on scientific commentary on the results. Details of the electronic papers (scheme, authors and a short synopsis of the results) are listed in the Table of Contents following the full-paper listing. Publication times for electronic papers are usually less than two months from submission to publication. It is anticipated that more authors will make use of the *Section C* electronic-paper submission route for rapid publication of their structural results without the need for any detailed discussion in the paper.

All *Section C* Co-editors had input into the revisions of the 2000 *Notes for Authors*; these were made with the intention of clarifying what is required for successful CIF submission to *Section C*. The full listing is available *via* the CIF help page at <http://journals.iucr.org/c/services/authorservices.html>. A detailed example of a CIF that meets all the *Section C Notes for Authors* requirements is also available at that site along with a new template that users of the popular *SHELXL97* refinement program should find useful, if they have not already developed their own CIF-making routines.

There have been several recent changes to the Editorial Board. C. Glidewell (U. of St Andrews), whose research interests lie in crystal engineering of molecular solids and organometallic polymers, is now the Deputy Editor. Co-editors A. Linden and A.J. Blake have become Data-Validation Editor and Deputy Data-Validation Editor, respectively. The team is completed by new Co-editors P.D. Boyle (North Carolina State U.), J.F. Gallagher (Dublin City U.) and N. Ishizawa (Tokyo Inst. of Technology).

George Ferguson, Editor



## Acta Crystallographica Section D: Biological Crystallography

1999 saw a number of major developments for *Acta Crystallographica Section D: Biological Crystallography*. The monthly publication of the journal was a great success; the continued reduction in publication times attracted many excellent structural and theoretical manuscripts. In addition to the research papers, crystallization papers and short communications, the journal has now seen the introduction of new sections of new commercial products, recruitment and meetings. The year also marked a redesign and the launch of the electronic edition of the journal as *Biological Crystallography Online*. Apart from providing the full text of the articles in the journal, this edition contains many additional features including linking to online databases such as the Protein Data Bank and Medline, and is continuing to develop to provide a complete service for biological crystallographers.

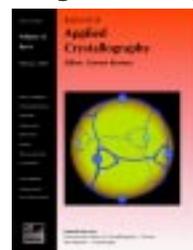
The IUCr has reviewed its policy on deposition and release of macromolecular coordinate and experimental data, and a set of guidelines has been published [*Acta Cryst.* D56 (2000), 2]. *Acta Crystallographica Section D: Biological Crystallography* will follow the recommendations given in these guidelines and urges other publishers to do likewise. Other supplementary material for a paper, for example diagrams and mathematical appendices, can be deposited in the IUCr electronic archive for retrieval online.

Since 1998, the journal has been the home of the popular proceedings of the CCP4 (Collaborative Computational Project No. 4 in protein crystallography) annual study weekends. The theme of this year's issue, which will appear in the summer, is low-resolution phasing.

We are pleased to welcome the Past President of the IUCr as Co-editor; Ted Baker (U. of Auckland), who has wide experience in protein structure analysis, notably of metalloproteins, also has interests in structural genomics, mutagenesis and protein engineering. It is the wide-ranging expertise of the Editorial Board that maintains the balance between high-precision information and analysis of results in terms of biomolecular structure and function.

Jenny Glusker, Editor

## Journal of Applied Crystallography



The *Journal of Applied Crystallography* is dedicated to the dissemination of all crystallographic work related to applied sciences, embracing experimental, technical,

theoretical and numerical/computing aspects. Apart from regular Research Papers, (invited) Lead Articles, Short Communications and Fast Communications, special sections are devoted to Laboratory Notes, Cryocrystallography, Computer Programs and manuscripts on Teaching and Education. Book Reviews, news of Crystallographers, notes on New Commercial Products and a Calendar of Events complete the set of subjects. The current success is the result of Michael Glazer's nine years of service as Editor. He assembled a fine group of Co-editors and topical Editors to assure expert service to the broad community of authors and readers.

I was fortunate to take over a well-functioning operation in 1999. I have been a Co-editor from 1980 to 1989 already and an occasional Guest Editor for the proceedings of the triennial conferences on small-angle scattering, a field in which I have been active for almost 30 years. My interest and experience in defects and phase transformations in inorganic materials and in crystallographic techniques (using X-rays, neutrons and electrons) will be a good basis for my dedicated attention to the matters of the *Journal of Applied Crystallography* and for maintaining its high scientific standards.

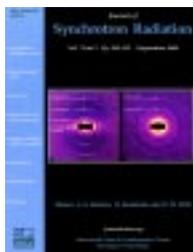
With the first issue of Volume 33 (February 2000), the *Journal of Applied Crystallography* changed its format and overall appearance to adopt a more modern look and layout. The keywords printed on each cover will be selected to reflect the variability of content for this particular journal.

After the major changes in appearance and the introduction of online services and other electronic publishing tools, no dramatic changes are planned for the next few years. The use of modern electronic means of submission, production, checking and dissemination offers new possibilities for the presentation of scientific results. Authors, readers and editors will have to learn how to use the electronic media efficiently

and skillfully. The possibility of offering online features within an article should be fully explored but should not lead to a loss of quality, be it electronic or printed material. A good journal is not just a list of links to electronic sites. Peer assessment will remain the major mechanism of assuring the quality of scientific publications, as long as there are readers (and authors) who recognize "the difference". In every self-organizing system, the balance between agitation and relaxation on various scales will decide on the overall properties. For the scientific community in general, exchange of ideas and know-how is crucial and must remain feasible (and manageable) on as many "scales" as possible. A good *Journal of Applied Crystallography* with all its related activities will continue to serve its purpose.

Gernot Kostorz, Editor

IUCr journal Editors and Co-editors (identified below with titles, initials and surnames) and Chester editorial staff (identified by first names and surnames) at the JComm meeting in Manchester in August 1999. Back row: Dr H.M. Einspahr, Dr W.C. Stallings, Dr M.R. Taylor, Michael Hoyland, Sean Conway, Brian McMahon, Prof. G. Kostorz. Fourth row: Nicola Ashcroft, Gillian Holmes, Dr F.R. Fronczek, Prof. D. Schwarzenbach, Dr A. Oskarsson, Prof. Y. Ohashi, Prof. D. Pandy, Prof. I.D. Brown, Dr C.J. Howard, Amanda Berry. Third row: Andrea Sharpe (Promotions Officer), Louise Clark-Jones, Katie Moore, Sue King, Prof. C.E.P. Lecomte, Prof. M. Vijayan, Prof. A. Kalman, Dr A.M. Moore, Dr M.J. Adams, Prof. G.R. Desiraju, Prof. G.B. Jameson, Dr M.M. Harding, Jill Bradshaw. Second row: Prof. J. Vicat, Dr A.L. Spek, Prof. G. Ferguson, Dr A. Linden, Dr A.J. Blake, Prof. W. Clegg, Peter Strickland, Prof. C.P. Brock. Front row: Prof. A.M. Glazer, Dr J.P. Glusker, Prof. S.R. Hall, Prof. J.R. Helliwell, Dr F.H. Allen, Prof. A. Authier.



## Journal of Synchrotron Radiation

In the six years since the *Journal of Synchrotron Radiation* (JSR) was launched, we have published about 870 research articles in nearly 4000 pages. Our aim has been to provide a focus for the whole of the synchrotron radiation community, and to publish high-quality papers covering sources, instrumentation, methods and applications for all regions of the synchrotron radiation spectrum. A major development for JSR has been the introduction of Synchrotron Radiation Online, an electronic journal service with many exciting features.

The journal has published the proceedings of two major conferences, SRI'97 (May 1998 issue) and XAFS X (May 1999 issue), and will cover XAFS XI in 2001. A dedicated issue on structural biology in July 1999 marked the first Nobel prize for synchrotron-radiation-based work, awarded to Sir John Walker of the MRC's Laboratory of Molecular Biology. The issue included several excellent articles from the leaders in the field demonstrating the transformation in structural biology brought about by synchrotron radiation.

Special issues are an important part of increasing the impact of the journal, its distribution and readership. Indeed, JSR now ranks in the top 17% of the Science Citation Index of 4800 journals. Its impact factor increased by 32% from 1996 to 1998 and it already ranks 3rd out of 52 journals in the instruments and instrumentation field. This is due to the excellent quality of papers submitted by authors, and care exercised by our referees.

A recent addition to the Editorial Board is H.A. Padmore (Advanced Light Source, Lawrence Berkeley National Lab). Dr Padmore's major contributions to synchrotron radiation have been in the area of instrumentation, notably soft X-ray monochromators, mirror systems for microfocusing, photoemission electron microscopy for investigating the magnetic structure of surfaces, and the utilization of low-energy storage rings for hard X-ray experiments. In September, Co-editor D.M. Mills will succeed J.R. Helliwell as JSR Editor. Dr Mills is currently the Director of the User Program Division of the Advanced Photon Source (APS) at Argonne National Lab and Executive Director of the Synchrotron Radiation Instrumentation Collaborative Access Team (SRI-CAT). He has spent the last 25 years developing instrumentation for use with synchrotron radiation. His research interests include the application and use of the unique properties of synchrotron radiation to studies of X-ray physics, in particular X-ray optics, and time-resolved experimentation.

JSR has clearly become established; our goal now is to increase the number of subscribers. If your library does not already subscribe, please encourage them to do so, so that the work of the synchrotron radiation community – from "source to science" – can reach the widest possible audience.

Samar Hasnain, John Helliwell and Hiromichi Kamitsubo, Editors





## More Reports from Glasgow

(see also Volume 7, No. 4 pp. 6-14)

### Bragg Lecture

The 1999 Bragg lecture entitled "Polymorphism; The Same yet Different" given at the Glasgow IUCr Congress by Jack Dunitz, ETH, Zurich reflected the change in outlook of chemists towards polymorphs during his lifetime, from an unwanted nuisance to a thriving research field. Prof. Dunitz suggested that the impetus for this change of attitude came from the challenge of crystal engineering in the pharmaceuticals industry, and the need to predict crystal structures and molecular properties.

He related the "Strange Case of the Disappearing Polymorphs". This ability for one thermodynamically stable form to dominate over another polymorph can have important implications for the pharmaceutical industry, especially when litigation and a lot of money is involved.

Based upon examination and analysis of many polymorphs, Dunitz has concluded that "The optimal packing of a collection of identical molecules necessarily leads to the densest packing".

Pam Thomas, *BCA Newsletter*, Sept. 1999

### Real Time *in situ* Reaction Chemistry

Highlights of this session included H. Uekusa's analysis of an unknown crystal structure using intensity data collected in 17 seconds with the newly developed MSGC detector, P. Coppens' description of the determination of light-induced transient species of a series of coordination compounds and Ohashi's detection of several light-induced metastable species of organic compounds.

Yuji Ohashi

### Structural Enzymology

The microsposium focused on enzymes that utilize unusual cofactors. J. Fontecilla-Camps discussed hydrogenases containing Fe in their active site or a combination of Fe and Ni coordinating CO, CN or cysteine thiolate. The function of the metal ions was discussed with emphasis on the spin state of Fe. The diffusion of H<sub>2</sub> through long channels in the proteins was beautifully illustrated by loading them with Xe.

C. Wilmot showed snapshots of the reaction pathway of an amino oxidase which utilizes Cu and 2,4,5-trihydroxyphenylalanine quinone as cofactors. Individual steps of the reaction were flash-frozen and analyzed at high resolution. The quinone "jumps" from one step to the next in the reaction cycle and, surprisingly, O<sub>2</sub> was seen to bind to Cu prior to oxidizing amine to the corresponding aldehyde.

U. Ermler described methyl-coenzyme M reductase, a 300 kDa heterohexamer catalyzing the last step of methane metabolism. This step involves the oxidation of coenzymes M and B to a heterodisulfide with the cooperation of coenzyme F<sub>430</sub> containing a Ni-porphinoid and transient formation of radicals and a Ni-Methyl complex.

Another multistep reaction, presented by K. Brown, concerned a Zn and NAD<sup>+</sup> containing 3-dehydroquinase synthase in the shikimate pathway. The enzyme catalyzes alcohol oxidation, carbonyl reduction, ring opening, phosphate β-elimination, and intramolecular aldol condensation. Knowledge of the architecture of the active site will be of interest for drug design since several parasites,

but no mammals, use this pathway.

A movie produced by A. Anderson showed clearly the reasons for anticooperativity in the homodimeric thymidylate synthetase enzyme. In complex with substrate dUMP and cofactor analog CB3717 the homodimer is asymmetric, binding two molecules of the former but only one of the latter. The reason for anticooperativity is seen in covalent bond formation between the catalytic cysteine and dUMP in one subunit that induces a conformational change in the other and prevents such bond formation.

A. Becker presenting the acetyl-CoA synthesizing enzyme pyruvate formate-lyase, a 340 kDa homodimer. In the reaction, a pyruvate bond is cleaved utilizing a free and stable radical located at Gly734. There is no metal ion involved in radical formation, contrasting with other known enzymes that engage Fe (III).

W. Saenger

### Endocytosis and Exocytosis

Dramatic progress has been made to elucidate the structures of key components of membrane vesicular traffic, including those responsible for calcium-triggered neurotransmitter release, protein secretion, and hormone release. R.B. Sutton presented the structures of the synaptic fusion complex (a SNARE complex prototype) and the calcium sensor synaptotagmin. The free energy released by the assembly of the SNAREs probably leads to eventual fusion of the vesicle and target membrane. W.I. Weis presented the structures of the D2 and N-terminal domains of N-ethylmaleimide-sensitive factor (NSF) (these two domains were solved independently in the Weis and A. Brunger laboratories) and proposed a mechanism for its function. NSF is an ATP-driven chaperone that dissociates the SNARE complex so that its components can engage in another fusion cycle. Equally dramatic progress has been made to elucidate the structures of proteins involved in vesicle formation and cargo selection during clathrin-mediated endocytosis. Clathrin is recruited to the plasma membrane, where it forms the coat that drives vesiculation and recruitment of the adaptor molecules that capture transmembrane receptors. E. Ter Haar presented the peptide-in-groove model to describe the structure of complexes between the N-terminal domain of clathrin and the clathrin-box binding motifs responsible for the recruitment of the adaptors to the clathrin coat. P. Hwang discussed the structure of a leg-segment of clathrin. P. Evans presented structures of several domains of the endocytic adaptor AP-2 complex. The m2 domain structure was solved in complex with peptides corresponding to the tyrosine-based sorting signals of



Speakers from the Endocytosis and Exocytosis Left to right: Tom Kirchhausen, Phil Evans, Bryan Sutton, William Weis, Martin Lawrence, Axel T. Brunger, Peter Hwang, Ernst ter Haar.

a number of proteins and a general model for recognition was presented. The transferrin receptor is recruited by AP-2 adaptors and undergoes multiple rounds of clathrin-mediated endocytosis to import iron-loaded transferrin and is also a key component in human hereditary hemochromatosis, a prevalent genetic disease. M. Lawrence presented the structure of the complete ectodomain of human transferrin receptor and proposed a model to explain the recognition of transferrin by its receptor.

Axel T. Brunger and Thomas Kirchhausen

## Crystal Engineering

J. Atwood kicked off the microsposium with an exhilarating journey into the world of supramolecular synthesis. Using one of the 13 Archimedean solids, the snub cube, as a topological target, he described the synthesis of calixarene based structures. Hydrogen bonds and electrostatic interactions were used to construct and control complex nanoscale assemblies. The focus then shifted in I. Dance's presentation to the interactions themselves. Dance described hexaphenyl and tetraphenyl embrace motifs which are co-operative C-H... $\pi$  based patterns, associated with at least 10 kcal/mol stabilisation. These motifs may be employed reliably in crystal engineering. Dance pointed out that inorganic and organometallic structures wherein the tetraphenyl phosphate cation is commonly used have greater diversity than organic molecular solids.

After witnessing the solar eclipse, the congregation reassembled to hear Y. Aoyama's thought-provoking talk on spontaneous resolution. Although this phenomenon is well-known, it is poorly understood. Aoyama addressed issues such as relationship of molecular structure to spontaneous resolution, theory of chirality and the possibility of employing spontaneous resolutions on a more general basis. B. Foxman followed with a summarising talk on reactive molecular crystals. He showed that solid state topochemical synthesis can extend beyond 2+2 cycloaddition reactions and gave several examples of thermally induced reactions, rearrangements and isomerisations.

The two final short talks by M. Jaskolski and M. Davidson, dealt with examples of weak or non-conventional C-H...X hydrogen bonding. Jaskolski chose meaningful examples from the biomolecular world mentioning C-H/N-H synthon interchangeability, C-H group acidity and cooperativity in nucleoside structures. In a brief but informative overview, Davidson showed examples of hydrogen bonding to highly activated carbon bases. In his well-illustrated talk, he pointed out that synthons based on these weak interactions control supramolecular structure effectively.

The microsposium showed how rapidly, and in how many directions this field is advancing, and how it offers tremendous scope to crystallographers and chemists alike. The growth of the field has produced two specialist journals, *Crystal Engineering* and *CrystEngComm*.

G.R. Desiraju

## Uses of the Inorganic Database

H. Behrens described the new arrangements under which the ICSD is being maintained by the Fachinformationzentrum Karlsruhe (Germany) with software by V. Karen (NIST, USA), and data validation by R. Allmann. S. Abrahams showed us how to find new ferroelectric materials by searching the ICSD for polar structures that are close to having a center of symmetry, and M. Berndt de-



Speakers in the session Crystal Engineering, (left to right) seated: Mike Zaworotko, Gautam Desiraju, and Robin Rogers. Standing: Yasu Aoyama, Jerry Atwood, Ian Dance, and Bruce Foxman.

scribed how a derived database of standardized structures can be used to find compounds with similar structures.

J. Rodgers talked about the CRYSTMET file of metal structures and M. Berndt described progress with the Pauling File which contains information on the structures and properties of binary compounds and will be extended to include all inorganic and metallic compounds by 2007. The Powder Data File (PDF) has been extended by including some 40,000 new powder patterns calculated from structures in the ICSD. J. Faber showed how to search this part of the PDF for groups of compounds that shared interesting properties, and A. Hewatt demonstrated his web version of the ICSD.

I. David Brown

## Perovskites

The main theme of the session was oxide materials with unusual electronic or magnetic properties. P. Bordet (CNRS, Grenoble) described structural anomalies at the superconducting transition in  $\text{HgBa}_2\text{CuO}_{4+d}$  from single crystal powder diffraction and EXAFS spectra. A general treatment of tilting in perovskites and a new computer program to derive the tilt systems was given by P. Woodward (Ohio State, USA). M. Fernandez-Diaz (ILL, Grenoble) reported a remarkable charge disproportionation coupled to a structural transition in the undoped lanthanide nickelate perovskites  $\text{LnNiO}_3$ . The session ended with two talks on layered manganite perovskites. J. Mitchell (Argonne, USA) showed how new CMR Ruddlesden-Popper phases could be prepared by controlling oxygen stoichiometry, and V. Caignaert (Caen) described the preparation of La/Ba ordered and disordered polymorphs of  $\text{La}_{0.5}\text{Ba}_{0.5}\text{MnO}_3$  and discussed their different physical properties. The session illustrated the continuing challenge to understand the relationships between composition, structure and properties in perovskite oxides.

J.P. Attfield and Juan Rodriguez-Carvajal

## Teaching Session

This session covered short courses and innovative teaching using the Internet or personal microcomputers. B-C Wang described an ACA course which includes 8 days of general crystallography with hands-on structure solving, followed by 4 days on the tech-

niques of crystallisation and structure refinement for macromolecules. K. Al-Sayed described a materials science course for M.Sc students given in Egypt.

D. Moss coordinated the development and use of several Internet based courses in structural molecular biology, beginning in 1996 with the 'Principles of Protein Structure'; a course on 'Powder Diffraction' is planned for October 1999. He highlighted the advantages and problems associated with teaching a world-wide class involving different time zones.

A. Fretwell spoke on the development of the MATTER project, now a set of some 30 modules on aspects of materials science available on CD-ROM, with an interactive demonstration of parts of the 'Crystallography' module. A Web based 'Diffraction' module is planned to be freely accessible on the Internet in October 1999.

R. Neder concluded the session with an interactive demonstration of his program using computer simulation as a teaching tool.

Kate Crennell and Karimat Al-Sayed

## Time-Resolved Crystallography and Protein Dynamics

The session ranged from X-ray crystallographic studies using 3D crystals and electron microscopic studies using 2D crystals to simulations and molecular dynamics calculations. G. Petsko (Brandeis U.) presented an overview of time-resolved crystallography, the methods for and problems with triggering reactions in crystals, the Laue method on fast time scales and slowing and trapping approaches. H. Kato (Kyoto U.) described a phosphorylation reaction of glutathion synthetase using photolysis of caged ATP to start the reaction. Time-resolved Laue and cryocrystallographic experiments were performed that showed the build-up of the phosphorylated transition state analog and the concomitant ordering of a loop. R. Henderson (MRC) used electron microscopy, photolysis and freeze trapping to look at the structures of reaction intermediates in 2D crystals of wildtype and a mutant bacteriorhodopsin. J. Hajdu (Uppsala U.) reported results obtained by an EU collaboration on the use of free electron lasers for structure determination. Simulations indicated that 10 fs pulse length might result in diffraction before the sample disappears in a plasma, whereas this seemed not to be true for 70 fs pulses. Protein dynamics were addressed by G. Bradbrook (Grenoble). The importance of water molecules and protons was taken up again in the summary of the session by J. Helliwell (Manchester U.) who also addressed the complementarity of neutron diffraction experiments with atomic resolution X-ray studies.

Ilme Schlichting

## Aperiodic and Incommensurate Structures

This minisymposium concerned with symmetry and theory included a discussion of random tiling theory treating diffuse scattering from phason fluctuations in a hydrodynamic approach (M. Widom); colour symmetry of aperiodic structures (R. Lifshitz); a reversible phase transition from a quasiperiodic to a periodic structure with tetrahedral symmetry (M. de Boissieu); and generalization of the symmetry concept to include general point sets, such as model and Meyer sets (D. Joseph). The most mathematical contribution came from J.-L. Verger-Gaugry, who showed calculation of the intensity of systems even in the case of a singular continuous



Teaching Session speakers (left to right) Seated in front: Karimat El-Sayed, Kate Crennell (session organisers). Standing: Reinherd Neder, Ann Fretwell (replacement for the Peter Goodhew listed in the program) David Moss, Hi-C Wang.

spectrum, and the power laws with which the intensity scales as a function of sample size.

T. Janssen

## Strong Closed-Shell Interactions

L.G. Kuz'mina (Russia) opened the microsposium with a discussion of the tendency of the Au(I) atoms to form clusters ( $d^{10}$ - $d^{10}$  interactions) and undergo interesting reactions in which the "strength" of these "weak" interactions was made evident. N. Runeberg (Finland) analyzed the contributions to the interaction energy between closed-shell centers, particularly  $d^{10}$  metal centers and concluded that the auophilic interaction is mainly a consequence of the dynamic electron correlation contribution strengthened by relativistic effects.

V.G. Tsirelson (Russia), and V. Luaña (Spain) discussed chemical bonding, instead of binding, using the concepts of the Atoms in Molecules theory. They showed experimental and calculated electron density maps of rare gases and of fully ionic compounds where closed-shell bonding occurs. They illustrated anion-anion and cation-cation bonding features.

A. Vegas (Spain) presented a comparison between the cation arrays of ionic solids and the structure of the corresponding metals. In an overwhelming number of ionic compounds, cations reproduce, both the topology and distances of the parent metal structure. They have been able to detect an empirical trend in the capacity of many atoms to form aggregates, in spite of having like charges.

A. Vegas and P. Pyykk

## Topography

J. Haertwig (Grenoble) surveyed the state of topographic imaging with third-generation synchrotron radiation at ESRF Grenoble, the various methods, their instrumentation, and applications to problems of solid state physics and material science. The high intensity of synchrotron radiation (up to 100 keV), and its large spatial coherence allow imaging by phase contrast radiography and (3D) tomography in a simple way.

Y. Epelboin (Paris) described "the topographic suite" of programs for the simulation of x-ray topographic images for various topographic

settings and optical characteristics of the radiation source.

The benefits of the long beamline (80 m) of the Topography Station at SRS Daresbury with its small vertical divergence for topographic reticulography were demonstrated by A.R. Lang (Bristol). In this method a fine absorbing mesh is placed behind the crystal and projected by the diffracted beam on a photographic plate with varying distance to the mesh. The distortions of the mesh shadow allow determination of the orientation differences between crystal segments of the probe. A reticulograph of a giant screw dislocation in SiC allowed determination of the handedness of the screw.

M. Dudley (Stony Brook) reported on white-beam synchrotron topographic studies of hollow-core superscrew dislocations in 4H- and 6H-SiC single crystals. A novel topographic procedure to determine the point-to-point lattice parameter variations near the crystal surface was introduced by A.E. Voloshin (Moscow). The method is based on computer processing of plane-wave topographs obtained with conventional X-rays and allows *d*-value mapping on large specimen areas with spatial resolution of 3-10  $\mu\text{m}$  and high sensitivity to lattice distortions. The technique was applied to the study of KDP-type crystals grown from aqueous solution.

The last contribution (N. Goswami, New Delhi) dealt with the conventional X-ray topography and high-resolution diffractometry study of coiled GaAs membranes produced for force sensor applications.



Speakers in the Topography session (left to right): Helmut Klapper, Niranjana Goswami, Alexey E. Voloshin, Michael Dudley, Yves Epelboin, Andrew R. Lang, Zhengwei Hu, Juergen Haertwig.

H. Klapper



Staff of the XVIII Congress, Glasgow.

## Difficult Structures

This session addressed problems that continue to challenge all aspects of crystal structure determination. R. Boese discussed how to get crystals of very low melting compounds and those which form plastic or glassy phases. W. Clegg discussed improving your chance of structure determination by gathering data with synchrotron radiation. R. de Gelder discussed novel ways to phase data that resist routine application by getting the maximum out of Karle Hauptman determinants.

The difficulty of validating results was discussed in S. Parkin's talk "Expansion of Global Validation Criteria to 3-D: The R-Tensor". He addressed various ways to detect possible errors in either data or structural results. A. Linden in "Difficult Structures: Making them Fit for the Chemist" gave some general advice on how to answer delicate questions so as to prevent the chemist from drawing incorrect conclusions and at the same time persuade the *Acta Cryst* Editor to accept the paper.

Paul T. Beurskens and David Watkin

## Charge Density Analysis

P. Coppens (New York) gave an overview of experimental aspects and T. Koritsanzky (South Africa) talked about refinement procedures. B. Iversen (Denmark) gave an account of multi-temperature studies and surprising behaviour in the ordering mechanism in a mixed valence iron compound. Only at near 10 K did it become possible to determine reliably the charge density distribution. The other speakers, A. Kirfel (Germany), M. Takata (Japan); N. Ishizawa (Japan), and V. Streltsov (Australia) described applications to chemical and physical problems. Results from synchrotron radiation facilities in the USA, Germany, France, and Japan were presented.

Finn Krebs Larsen

## Oxford Cryosystems Prize

Prize for the best poster associated with cryogenics was awarded to F. Wien for poster P08.01.003 "A portable Cryostream to transfer crystals".

Kate Crennell, *BCA Newsletter*

## Asian Crystallographic Assn Officers

President: ..... Y. Ohashi  
Vice-President: ..... J. Simpson  
Secretary/Treasurer: ..... Shih-Lin Chang  
AsCA-2001 is scheduled for 4 days during November 18-25,2001. The exact dates are yet to be finalized. The chairman of the Organizing Committee is M. Vijayan.



## British Crystallographic Assn Officers

(<http://gordon.cryst.bbk.ac.uk/BCA/>)

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Secretary ..... H. Muirhead  
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(<http://www.hwi.buffalo.edu/ACA/>)

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## Mineralogical Society of America Officers

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Councillor ..... J. Post

## Crystallography in...

### China

The Chinese Crystallographic Society is an academic organization for Chinese crystallographers, whose council is known as the China National Committee for Crystallography in the Int'l Union of Crystallography. Chair: N. Min, Vice-Chairs: D. Xian, W. Chang, S. Lin, Z. Mai, X. Jin. There are 360 members in the Chinese Crystallographic Society. The primary areas of crystallography are aperiodic crystals, biological macromolecules, crystal growth and characterization of materials, crystallographic computing, crystallographic teaching, electron diffraction, neutron scattering, powder diffraction, structural chemistry, synchrotron radiation, and XAFS.

Xianglin Jin

### France

The French National Committee for Crystallography is currently composed of chairman C. Lecomte, Nancy (charge density, small molecules, materials science, proteins), B. Capelli, Paris (crystal physics, material science), D. Louer, Rennes (powder diffraction, materials science) and D. Moras (bio-crystallography, genomics). The committee is linked to the IUCr and ICSU through the French Academy of Sciences. The board of the French Crystallographic Association (FCA) is composed of: chair, C. Lecomte, Secretary/Treasurer, B. Capelli, J.L. Hondeau (Grenoble) and A. Podjarny (Paris). The FCA has a general meeting every two years and the Biological group organizes an annual meeting. ECM19 and the FCA meeting for 2000 will be held simultaneously in Nancy, August 25-31. A crystallography school held in Toulouse in 1999 was attended by 10 students from Africa and 60 from France. Future schools for all French speaking students are planned for every two years. <http://www.lcm3b.u-nancy.fr>

C. Lecomte

### Israel

Israel Crystallography Association (ICA) officers are G. Shoham (Hebrew U.), Chairman; M. Kapon (Technion Haifa); Treasurer, M. Harel (Weizmann Inst.), Secretary. The ICA has 50 members and an annual meeting in May. Primary areas of research are macromolecular, surface, and small molecule crystallography and powder diffraction.

M. Harel

### Poland

The organizational structure of crystallography in Poland includes the Polish Crystallographic Society, the Polish National Committee on Crystallography, the Polish Society of Crystal Growth, the Polish Society of Synchrotron Radiation and the Polish Society of Neutron Diffraction. Almost all areas of crystallography are under study in Poland including chemistry, medicine, biology, organic compounds, metalloorganic, inorganic and intermetallic materials, protein crystallography, studies of crystal perfection and lattice defects, phase transitions in crystals at high and low temperatures, material science, powder methods, crystal growth, synchrotron radiation and neutron diffraction.

K. Lukaszewicz

### Serbia

The Serbian Crystallographic Society was founded in 1992 and has 50 active members. Officers of the Serbian National Committee for Crystallography are S. Stankovic (President), D. Poleti (Vice-President), Lj. Karanovic (Secretary), A. Kapor (Member), D. Rodic (Member), S. Trifunovic (Member), A. Kremenovic (Member). The Serbian Crystallographic Society hold an annual conference. Active areas of crystallographic research include investigations of structures of complex, inorganic and organic compounds, as well as minerals, magnetic structures and instrumental methods, and powder diffraction methods.

L. Karanovic

## Leiserowitz Still Cutting Edge

Leslie Leiserowitz was honored on his 65<sup>th</sup> Birthday with a symposium at the Weizmann Institute of Science. Leslie has consistently demonstrated the ability to identify challenging problems and the tenacity to find satisfying rational explanations. Speakers, P. Coppens, J. Als-Neilson, A. Gavezzotti and J.M. McBride described how Leslie's career, advice and collaboration had aided and inspired them in their careers. In his introductory remarks, M. Lahav said that when Leslie arrived at the Weizmann from South Africa he immediately applied the then very new Hauptman-Karle Method to a structure determination and characterized an interaction in a crystal structure that he felt demonstrative of an CH...O hydrogen bond. Philip Coppens described how he, Leslie and D. Rabinowitz began the very first charge density study using the Weissenberg camera that G. Schmidt brought to the Weizmann. Philip also described his latest studies using synchrotron radiation to examine electron density in the excited states of molecules. He identified as suitable candidates for this new technology; molecular excited states, photochemical electron transfer, and long-lived charge separated excited states and stressed the need for a national facility for time resolved X-ray diffraction.

Jens Nielson described state of the art studies of two-dimensional crystals generated in his elegantly designed Langmuir trough. Leslie and Jens are collaborating on experiments to probe formation of cholesterol crystals beginning with monolayers and elaborating on them. Angelo Gavezzotti has gained tremendous insight into the principles of molecular aggregation from the wealth of data in the CSD, but still finds the prediction of structure fraught with difficulty. He is exploring the insights that can be gained from dynamic calculations. Gavezzotti finds that dozens of crystal form of nearly equal energy are predicted for most single molecules, while only one form is usually crystallized. Coppens and Gavezzotti expressed concern that they were studying problems that were highly important but might not be solved in their lifetime. O. Livnah presented another puzzle with his observation that peptides of essentially random sequence induced aggregation of the erythropoietin receptor when rationally designed peptides failed to do so.

Mike McBride was pleased to find himself on the young people's portion of the program with Livnah and I. Sagi who showed wonderful electron micrographs of RNA helicase with clear, separate strands of DNA. Sagi seemed delighted to announce that she was too young to have any anecdotes about Leslie's early years.

McBride, closing the symposium with four great talks in one including a video of the dissolution of crystals, a walk in the sands of Palmore, and demonstration that a cleavage plane in a hydrogen bonded crystal will be parallel to the family of planes that intersects the fewest H-bonds.

At a dinner for friends, family and students, Leslie demonstrated his exceptional talents as a devoted grandfather and the Master of ceremonies, Bill James (U. Cambridge) reminisced about his sabbatical at the Weizmann.

William L. Duax

## School in India on Powder Diffraction

An Int'l School on Powder Diffraction (ISPD'98) held at the Indian Association for the Cultivation of Science in Oct. 1998 was sponsored by the IUCr, ICDD, and the Indian National Science Academy through its National Committee on Crystallography. There were 250 participants from all over India and abroad. K. Lal, gave the keynote address on materials characterization studies and multi-crystal diffraction.

There were nine technical sessions and Hands-on Computer Session in which faculty members explained program details to the participants. Philips and Bruker exhibited high-resolution instruments and Dr. Faber (ICDD) demonstrated the role of the powder database and ICDD activities. Programs were distributed free of cost to the participants.

S. P. Sen Gupta  
Secretary ISPD 98

## India-Italy Synchrotron Workshop

The Workshop, held in November 1998, was sponsored by the Dept of Science & Technology, Govt. of India and Ministry of Foreign Affairs, Govt. of Italy. 100 participants attended 11 technical sessions and poster sessions. Topics covered included: Surface Structures, Protein Crystallography, Soft X-ray Microscopy, X-ray Standing Waves, Photoemission and ESCA, High pressure XRD and Structure from Powders, EXAFS, SAXS, Novel Materials, etc. Italian scientists presented possibilities and future experiments at Elettra. Because Indian Synchrotron Facilities are under construction, this collaborative workshop opened up a new phase in Indo-Italy co-operation with implication for the future.

S. P. Sen Gupta

## Polish Drug Design

The Second Int'l Conference on Crystallography and Drug Design (CDD'99), an interdisciplinary meeting for scientists engaged in structural chemistry, modelling, intermolecular interactions and drug design, was held in May 1999 in Poland. Most lectures were presented by crystallographers to an audience of medicinal chemists.

In Poland, Medicinal Academies are separate from Universities and their chemistry oriented departments are engaged mostly in



Drug Design Conference

## MEETING REPORTS

new drug synthesis. With advances in computer aided drug design, the need for structural data has become more apparent, providing crystallographers with new opportunities for interdisciplinary work.

Among the speakers at the Second Conference on drug design, organized by the staff of the Technical U. of Łódź, were G. Desiraju, W.L. Duax, P. Murray-Rust, A. Kalman and S. Price. The Third Conference is planned in conjunction with ECM in Cracow (2001).

After the Conference, Bill Duax received a degree of *honoris causa doctor* from Technical U. of Łódź. The fruitful collaboration between Duax and crystallographers of the Technical U. of Łódź led by Prof. Galdecki begun 20 years ago has resulted in 31 joint publications.

Marek Glowka

### Supramolecular Chemistry, Moldova

The XIII International Conference "Physical Methods in Coordination and Supramolecular Chemistry" held in Chisinau (Republic of Moldova) Sept. 7–10, 1999 was organized by N. Gerbeleu (R. Moldova) and J. Lipkowski, (Poland).

Data derived from magnetic chemistry, resonance methods (NMR, ESR, Mossbauer spectroscopy, etc.), quantum chemical calculations, mass spectrometry, and X-ray crystallography were presented. 120 participants from Poland, Russia, Romania, Ukraine, Belgium, Bielorrussia, Canada, France, Germany, Italy, Yugoslavia, and USA attended the Conference.

J. Lipkowski (Poland) discussed interactions between solute and solvent that may be subdivided into two categories, localized interactions where the 'partner' species can easily be distinguished, and more extended general interactions. He noted that in the crystal structures of clathrate hydrates two different modes of hydration co-exist: hydrophilic hydration, in which water is H-bonded and hydrophobic hydration in which water molecules enclathrate lipophilic parts of guest moieties. I. Haiduc (Romania) gave examples of weak but additive interactions in element-organic compounds.

M. Fonari (Moldova) presented studies of antimony trifluoride complexes with classic and modified crown ethers, including organic/inorganic synthons with charge assisted by hydrogen bonding and central atom coordination.

Calixarenes have been synthesized in an enormous variety of ring sizes. V. Kravtsov (Moldova) and E. Weber (Germany) analyzed the structures of heterocalixarene solvent inclusion complexes, heterocalix[8]arenes composed of benzimidazol-2-one and the 1,3-phenylene components in an alternate cyclic arrangement form of *endo*- and *endolexo* singular and mixed inclusion complexes.

Other topics addressed included calix (n) pyrroles that complex anionic and neutral species (K. Swinska, Poland), stability in  $\text{SiF}_4\text{-H}_2\text{O}$  macrocycles (Y. Simonov, Moldova), enantioselective complexes of N-nitrosopiperidines with optically active guests (M. Gdaniec, Poland).

Ya. Voloshin (Russia) described clathratochelates of iron, ruthenium and cobalt  $\alpha$ -dioximes, as models of metalloenzymes (biomimetics), efficient catalysts for chemical reactions, and promising materials for molecular electronics.

N. Gerbeleu (Moldova) discussed 'Electron Impact Mass



Polish and Moldavian crystallographers on the day of Conference opening.

Spectrometry in Coordination and Supramolecular Chemistry Investigations", including the detection of the transition from the traditional coordination compounds to supramolecular systems in polynuclear copper carboxylates.

Other presentations included talks on electronic transfer in trimeric iron carboxylates (I. Ogurtsov, Moldova), cadmium selenide in ion-selective membranes (O. Bizerea, Romania), nanoperiodic structures and mesoporous molecular sieves functionalized by amine and Schiff-base metal complexes (A. Filippov, Ukraine), and Mossbauer spectra of europium complexes with different ligands (K. Turta, Moldova).

A. Gulya closed the Conference with a lecture devoted to late Professor A. Ablov (1907–1978), the originator of the world-known coordination chemistry school in Moldova.

The participants enjoyed excellent Moldavian food and sparkling wines and the magnificently picturesque 'Old Orhei' valley.

Kinga Suwinska, Yurii Simonov

### Bio-Crystallography near Berlin

The 2<sup>nd</sup> Heart of Europe Meeting on *Bio*-Crystallography in Lübben in the Spreewald south of Berlin September 30 - October 2, 1999 was organized by Y. Muller and U. Heinemann from the MDC in Berlin-Buch and sponsored by MarResearch, Nonius, and Oxford Instruments. The meeting provided a platform for young researchers to present their work in an informal workshop-like atmosphere. With a total of 54 participants from Berlin, Braunschweig, Halle, Hamburg, Jena, Poznan, Prague and Ceske-Budejovice. Thanks to the sponsors, stipends could be given to three students from the Czech Republic, Poland and Germany.

Selecting highlights from the many excellent presentations is difficult, but necessary (for additional details, see: <http://www.mdc-berlin.de/~crystal/heart/hec.html>). Highlights of the meeting included a description of innovative ideas and techniques in the field of cryo-crystallography by S. Panjikar (IMB in Jena). The guest speaker, V. Lamzin (EMBL) discussed electron density maps and their interpretation, with a focus on his ARP/wARP method. J. Brynda (Prague) presented crystals of crystallin which were removed from a patient's eye. The doctors brought the crystals to the crystallography group, where the structure was solved and the cause for the

formation of crystals *in vivo* determined. J. Müller (MDC in Berlin-Buch) talked about a complex between adrenodoxin and adrenodoxin reductase in a crystal form with a 600 Å long cell axis. C. Betzel reported on the current status of the joint IMB Jena/U. of Hamburg/EMBL-beamline at the DESY synchrotron in Hamburg, and T. Knöfel (Free U. of Berlin) described an unusually large domain rotation upon activation of a 5'-nucleotidase. Finally, M. Wahl (FMP in Berlin) presented the structure of an NADPH-oxidase signalling domain. Martin, an NMR spectroscopist, experienced difficulties in trying to solve the structure by NMR, went to the crystallography group at the MDC in Berlin, crystallized the protein and the Se-Met protein, and solved the structure.

Mariusz Jaskolski from the CBB in Poznan and his group will organize the 3<sup>rd</sup> Heart of Europe Meeting on *Bio-Crystallography* in the fall of 2000.

Manfred S. Weiss



## Pittsburgh Diffraction

The 57th annual Pittsburgh Diffraction Conference was held in October in Columbus, OH, USA to honor Muttaiya Sundaralingam, Professor of Chemistry and Eminent Scholar at Ohio State U. on the 40th anniversary of his arrival in Pittsburgh to begin graduate studies in X-ray Crystallography. He has made many contributions to our understanding of structure and function in nucleic acids and proteins, at first with small molecules and then with macromolecules.

The scientific program included a symposium entitled "Physical Properties of Protein Crystals", organized by G. DeTitta and a symposium honoring Sundaralingam entitled "From Nucleic Acids to Proteins" organized by M. Caffrey and B. Craven. For detailed coverage of the meeting, see the ACA Newsletter, Summer 1999 (<http://www.hwi.buffalo.edu/ACA/Society-Info/Newsletter-1999summer/pg01.html>).

Bryan Craven, ACA Newsletter, Summer 1999

## Society of Japan Annual Meeting

The 1999 annual meeting of the Crystallographic Society of Japan was held in Kyoto, Japan in November. Three major sessions were concerned with instrumentation and data collection, materials research, and macromolecular structures. The eight talks on the methods session included recent advances in imaging plate detectors, vacuum camera imaging, density modification methods and Rietveld analysis. New studies of magnetic fluids (K. Ueda), alloys (M. Uchida), zeolites (K. Nakamura), GaN films (T. Koyama), special  $\text{LiMn}_2\text{O}_4$  (T. Kanbe), buried oxide layers of low-dose SIMOX wafers (T. Shimura), and domain structure of  $\alpha\text{-Al}_2\text{O}_3$  (Y. Nakakita) were described in the materials session. Recent macromolecular structures discussed included a Cu/TPQ containing amino oxidase (M. Kim), human hematopoietic prostaglandin D synthase (N. Okazaki), aspartate aminotransferase from *R. meliloti* (T. Nakai), L-histidinol phosphate aminotransferase from *E. coli* (K. Haruyama), pectate lyase from *B. subtilisin* (M. Akita), L-methionine from *P. putida* (H. Motoshima), 64M-5 antibody fab complexed with (6-4) photoproducts (N. Hayashida), and DNA duplex containing  $N^4$ -methoxycytosine adenine base pair (T. Hikima). Sixty-six posters



Participants at the 2<sup>nd</sup> Heart of Europe Meeting on *Bio-Crystallography* in September.

covering all areas of crystallography were also presented. The chairman of the organizing committee was K. Miki and program committee members were Y. Higuchi (Chair), S. Sasaki, Y. Noda, and M. Yasui. A list of the titles and authors of all presentations can be found at <http://wwwsoc.nacsis.ac.jp/crsj/index-e.html>.

Y. Noda

## Aminoff Prize Awarded

The Royal Swedish Academy of Sciences has awarded the Gregori Aminoff prize in crystallography for 1999 to Dr. Richard Henderson and Dr. Nigel Unwin, MRC Lab of Molecular Biology, Cambridge, England, for their development of methods for structure determination of biological macromolecules using electron diffraction. The prize was presented at the Annual Meeting of the Academy, March 31, 1999. A symposium entitled *Structure Determination of Macromolecules with Electron Diffraction* was held March 29-30 to honor the prizewinners. The symposium was supported by the Academy through its Nobel Inst. for Chemistry.

Lectures were given by the following invited speakers: R. Henderson (Atomic Resolution Electron Microscopy in Biology), N. Unwin (The Acetylcholin Receptor Channel – Approaching Atomic Resolution), H. Cheng (Virus Studies, Essence of Supermolecular Symmetry), H. Herbert (Electron Crystallography of Membrane-bound Enzymes), M. van Heel (Structure and Function of the Ribosome by 3d Cryo-EM), S. Hovmöller (Im-



Speakers at the The Royal Swedish Academy of Sciences Annual Meeting From left to right: So Iwata, Marin van Heel, Richard Henderson, Matti Saraste, Ivar Olovsson, Ulf Skoglund, Nigel Unwin, Hans Herbert, Werner Kühlbrandt, Sven Hovmöller, Michael Rossmann, and Holland Cheng.

aging Individual Atoms by Electron Microscopy), S. Iwata (Structural Studies on the Cytochrome bc1 Complex), W. Kühlbrandt (Making Light Work – The Membrane Proteins of Plant Photosynthesis), M. Rossmann (Where Electron Microscopy Meets with Crystallography), M. Saraste (Different Methods for the Study of Membrane Structures), U. Skoglund (Visualization of Single Protein Molecules by Electron Tomography).

*Ivar Olovsson, Chairman, Swedish Nat'l Committee of Crystallography*



## MSA Awards

**Ikuo Kushiro** was awarded the Roebling Medal, the highest honor given by MSA, for exemplary studies in experimental petrology.



**R.A. Howie** received the Distinguished Public Service Award for years of tireless abstracting. As principle Editor of Mineralogical Abstracts, he

continues to write some 1600 abstracts each year and also edits and proof-reads all 4500/5000 abstracts published annually.



**Yingwei Fei** received the Mineralogical Society of American Award for outstanding research early in a career. He is developing multianvil apparatus and diamond-anvil cell high-pressure techniques.

MSA cited **George D. Guthrie** and **Donnal L. Whitney** as the 1998-1999 MSA distinguished lecturers. The MSA sponsored lecturers travel from September through April giving talks at colleges and universities in the US and Canada about new directions of mineralogy. George Guthrie (Los Alamos Nat'l Lab) offered lectures on "Mineralogy in the lung, Geochemical mechanisms of mineral induced disease; London Bridges falling down?" Donna Whitney (U. of Minnesota-Minneapolis) offered "Petrology and global warming: How igneous and metamorphic processes change world climate"

## Congratulations to...

**Andrew Taylor**, Director of ISIS since 1993, on the award of an OBE for 'services to neutron scattering'.

**Mark Harris** (Rutherford Appleton Laboratory) received the 1999 Philips prize during the Closing Ceremony at the IUCr XVIII in Glasgow. It was given for his work in the field of magnetic frustration and, in particular, for his work in the area of magnetic pyrochlores.



**Judith Howard** (U. of Durham) received a £100,000 grant from the Wolfson Foundation of the Royal Society and the award for structural chemistry honoring her pioneering work of x-ray and neutron diffraction for locating hydrogen atoms in the presence of heavy metals. The grant will be used to create a bioinformatics centre. She also received a EPSRC senior fellowship award which allowed her to take a five-year sabbatical from teaching duties to do research. Alan Leadbetter commented "...she does too many things - but she does them all well".

**Frank C. Hawthorne** (U. of Manitoba) was awarded the 1999 Past-Presidents' Medal of the Mineralogical Assn of Canada.

ILL welcomes its two new associate directors, **Colin Carlile** as head of the projects and techniques division and **Christian Vettier**, head of the science division.

In 1973 **Alexander Rich**, a professor at the Massachusetts Inst. of Technology produced the first X-ray crystallographic structure of a double helix with atomic level resolution for his half century of probing the structures of DNA and RNA. Alex has been named the recipient of the \$250,000 Bower Award for Achievement in Science from the Franklin Institute on Philadelphia.

**Ian K. Robinson** of the U. of Illinois at Urbana-Champaign was chosen to receive the 2000 B.E. Warren Award from the ACA for his innovative application of diffraction techniques to the study of crystal surfaces. Since his earlier discovery of the importance of crystal truncation rods for understanding surface structure, he has continued to introduce new ideas for the physics of surface structures and transitions, including the recent use of reflectivity measurements with coherent X-rays to obtain a new kind of information about crystal surfaces. The award will be presented to Dr. Robinson at the ACA Meeting in St. Paul in July.



**Lyle Jensen** has been named the recipient of the Buerger Award of the ACA for 2000. Dr. Jensen's attention to detail, his understanding of the fundamentals of crystallography (exemplified by his well-used textbook), and his utmost faith that an experiment could be and should be carried out to the precision the method was capable of, are what underlie his ground-breaking work in finding hydrogen atoms, in proving that protein structures could be refined and in providing good phase information. Dr. Jensen will receive his award at a ceremony at the ACA meeting in St. Paul in July.



The American Chemical Society Division of Biological Chemistry presented awards at the 1999 ACS national meeting to **David S. Eisenberg**, professor of molecular biology and chemistry at the U. of California, Los Angeles, received (the Repligen Award); and **John Kuriyan**, who is Patrick E & Beatrice M Haggerty Professor at Rockefeller U. as well as a Howard Hughes Medical Inst. investigator, (the Lilly Award). Eisenberg has focused on the relationship of protein sequence to three-dimensional structure and function profile methods for describing a family of amino acids sequences and the field known as threading or fold prediction. Kuriyan's research concerns the atomic level mechanisms of intracellular signal transduction and the process of chromosomal DNA replication.



**Brian W. Matthews** (U. of Oregon and Howard Hughes Medical Inst.) is the recipient of the 2000 Stein and Moore Award from the Protein Society, which is sponsored by the Merck Foundation, for his pioneering contributions to X-ray crystallographic methods, protease structure, gene regulation and mutational analysis of protein stability. The award will be presented at the 14th Annual Symposium in San Diego, August 5-9, 2000.

## MSC Future Investigator Awards

Molecular Structure Corp. announces the creation of a new award to foster excellence in research from young structural biologists. To be eligible for the award, the participant must currently be employed as a postdoctoral fellow in the field of macromolecular crystallography with the intent to remain in the field on a permanent basis. The awards are open to applicants from anywhere in the world.

Four unranked MSC Future Investigator Awards will be announced on July 1. Each award carries an unrestricted cash prize of \$2500. To apply for the award, send a cover letter, CV, and copies of two recent publications to Dr. James Pflugrath, Molecular Structure Corp, 9009 New Trails Dr, The Woodlands, TX 77381 USA. The submission deadline is May 1, 2000. A committee will select Future Investigators based on a number of criteria, including the applicant's potential to make a positive impact on the field of structural biology.

## Table-top Picosecond Sources

A paper by C. Rose-Petruck *et al.*, *Nature* 398, 310-312 (1999) brings together X-ray diffraction and picosecond ultrasonics. X-ray pulses with tens of picoseconds to nanosecond duration were used to study shocked and annealed crystals and photo-initiated reactions within proteins. The picosecond X-ray barrier was broken following rapid developments in high-power laser technology.

Rose-Petruck *et al.* describe the generation of picosecond bursts of copper  $K_{\alpha}$  radiation by irradiating a thin copper wire with a short-pulse high-power laser. This ultrashort radiation is used to measure the response of a gallium arsenide (GaAs) crystal to sudden heating. This did not require a large facility and uses equipment of a cost and scale commensurate with the ambitions of a well-equipped university department. It may ultimately allow changes in electron density to be monitored during biological and chemical reactions, with femtosecond resolution.

*Nature*, Vol. 398, March 1999

## Spo0F Proof?

Tired of the reliable but presumed static data on macromolecules provided by X-ray analysis? Biochemists are using NMR dynamics studies to probe relationships between molecule movement and function. Feher and Cavanagh, [*Nature*, 400, 289-293 (1999)] detect amino acid residues moving on a microsecond to millisecond timescale in a protein involved in a phospho-relay signal transduction pathway in *Bacillus subtilis*. The moving residues correspond to amino acids previously identified as important in mediating interaction with three signaling partners. Is there a hidden significance to the fact that the acronym for the protein under study is known as Spo0F?

## Duh, Even Blondes Won't Apply

Netherlands Organization for Scientific Research (NWO) show that last year it filled less than a fifth of postdoctoral positions within its program grants. Recruitment difficulties are due to a variety of factors, he continues, most importantly a **lack of career development and prospects**. Postdocs want permanent positions.

*Nature*, Vol 403, January 2000

## AACG Begins Yearly Meetings

The Executive Committee of the American Association for Crystal Growth (AACG) has decided to begin holding its meetings every year on a trial basis. Traditionally AACG has held a national meeting every three years. In 2000 a national meeting has been scheduled for Vail, a popular site where AACG members have gathered in the past and bids for a East Coast site for 2001 are under consideration. The AACG co-sponsored the 1999 ACA meeting in Buffalo and the ACA has discussed joint meetings in the future.

## MSA 2001 Grant for Research

A \$3,500 grant in support of research will be made in January, 2001 by the Mineralogical Society of America. Application forms for the grant may be obtained from the MSA web page, [http://www.minsocam.org/MSA/Grant\\_Appl.html](http://www.minsocam.org/MSA/Grant_Appl.html). Applications must be returned by June 1, 2000.



## Australian Synchrotron Research Program (ASRP)

The expansion of the ASRP into the Advanced Radiation Source (APS) in Chicago now gives Australian researchers access to third generation synchrotron radiation. Visit the following web sites for

more information:

- [www.ansto.gov.au/natfac/asrp.html](http://www.ansto.gov.au/natfac/asrp.html) - for an overview of the ASRP
- [www.aps.anl.gov](http://www.aps.anl.gov) - for an overview of the APS in Chicago and links to all its CATs
- [cars1.uchicago.edu/chemmat/chemhome.html](http://cars1.uchicago.edu/chemmat/chemhome.html) - overview ChemMatCARS CAT
- [cars1.uchicago.edu/biocars/biocars\\_home\\_page.html](http://cars1.uchicago.edu/biocars/biocars_home_page.html) - overview BioCARS CAT
- [www.aps.anl.gov/sricat/](http://www.aps.anl.gov/sricat/) - overview SRI-CAT

**ChemMatCARS** is devoted to the study of chemistry and materials science. •Single crystal crystallography, •High energy resolution XAFS, •Static and time-dependent reflectometry on liquid and solid surfaces, •Static and time-dependent small and wide angle X-ray scattering (SAXS /WAXS) on liquids and 'soft' solids such as polymers and fibers.

**BioCARS** has three separate beam lines devoted to protein and virus crystallography: SRI-CAT (Sectors 1 to 4) for (1) Time resolved, high-energy X-ray, and high heat load studies; (2) X-ray microprobe, high-resolution soft X-ray spectroscopy, and deep X-ray lithography; (3) Inelastic X-ray and nuclear resonant scattering studies; and (4) Polarization/magnetic studies.

## Curtin U. of Technology, Dept of Applied Physics

The crystallographic laboratory is one of the principal facilities of the Curtin Materials Research Group which specializes in industry-directed research. Principal focus is upon Rietveld analysis and the development of procedures to measure absolute phase abundance, texture, strain, crystallite size, etc. Extensive use is made of neutrons (MRPD and HRPD powder instruments at Lucas Heights), and synchrotron radiation (BIGDIFF at the Photon Factory, Tsukuba, Japan) to supplement laboratory-based X-ray diffraction measurements.

## More Structural Biology at St. Vincent's

Study of Structural Biology at St. Vincent's Institute of Medical Research in Melbourne, Australia was expanded in 1997 following the Wellcome Trust-supported appointment of Bostjan Kobe as Head. The focus of the Lab are studies of macromolecular interactions, using a combination of protein chemistry, molecular biology, the biosensor and computational approaches, in addition to macromolecular crystallography. The biological areas under study include regulation of protein function, viral infection, cellular transport processes and protein-protein interactions. Recent research highlights include the determination of crystal structures of the autoregulated proteins phenylalanine hydroxylase, importin  $\alpha$ , and the HTLV-1 virus envelope glycoprotein gp21 as a chimera with maltose binding protein. A portion of equipment was set up through the efforts of Michael Parker and Bruce Kemp. Some facilities are shared between the Structural Biology Unit and the Ian Potter Foundation Protein Crystallography Unit headed by M. Parker.

Bostjan Kobe

## CIF NEWS-4

The Crystallographic Information File (CIF) and its macromolecular extension (mmCIF) have become foundations for two key crystallographic resources, *Acta Crystallographica C* and the Protein Data Bank (PDB). The Powder Data File and the Inorganic Crystal Structure Database are also in the process of adopting CIF to represent experimental and structural information. The modelling and NMR communities plan to use CIF. CIF permits detailed description of each aspect of an experiment and its results in a computer readable form.

Although the structure of CIF is essentially very simple, the details can prove confusing to new users. Three of the most frequently asked questions are:

### 1. How are CIF data names chosen?

Each data name in CIF has to be unique so that a computer knows exactly what the data value represents. This leads to names, such as `_atom_site_fract_x`, that are composed of several familiar words or their abbreviations. Since a data name cannot include blanks (these are used to terminate the name), the individual elements are linked by underlines. Any character string starting with an underline could serve as a data name, but the names have been chosen so that users can see the underlying structure of the file: the names of related items start with the same string of characters. These relationships are coded into the dictionary in a rigorous way.

### 2. Are there user interfaces for CIF?

The web based input tool used by the Protein Data Bank is actually an editor for mmCIF, the macromolecular extension of CIF. This tool allows users to type in the required information and provides simple pull down menus for many of the data items. An editor for the core CIF used by *Acta Crystallographica C* is in preparation.

### 3. I am writing software and need an item not defined in any CIF dictionary. What can I do?

In the short-term you can define local data names for items and include them in a CIF. The data item must follow the CIF syntax and must not duplicate an existing CIF data name. This can be achieved by incorporating a distinctive string (such as the name of the laboratory) into the data name. One of the CIF syntax rules is that a program should ignore any data item whose name it does not recognize. Thus the presence of a local data name will not invalidate the CIF and will not prevent it being read by other programs.

If your programs or files are distributed to other laboratories, you may wish to register a local prefix with COMCIFS, the committee responsible for the maintenance of the CIF standard. This prefix would appear as the first element in any data name defined in the local dictionary. If the prefix is registered, a user can then track down the local dictionary. In the future, applications will automatically be able to locate a registered local dictionary on the web and transparently concatenate it with the CIF dictionary currently being used. To register a local dictionary name contact Brian McMahon at [bm@iucr.org](mailto:bm@iucr.org).

If the new data item is likely to be of more general interest, it should be added to one of the CIF dictionaries. In this case, you should contact the appropriate Dictionary Management Group (David Brown at [idbrown@mcmaster.ca](mailto:idbrown@mcmaster.ca) for the core dictionary, Helen Berman at [berman@rcsb.rutgers.edu](mailto:berman@rcsb.rutgers.edu) for the macromolecular dictionary and Brian Toby at [brian.toby@nist.gov](mailto:brian.toby@nist.gov) for the powder dictionary). They will be able to advise on the procedure for creating a new CIF data name. Contact David Brown or Brian McMahon if you are not sure which dictionary is appropriate.

I.D. Brown

## General Utility Lattice Program

This is a program for the simulation of solids, molecules and defects using interatomic potential models. Originally designed for the modelling of ionic materials and incorporating the shell model for ionic polarization, GULP now contains all the functionality required to treat more general systems such as biological molecules and metals. The program is available to academics at no charge for non-commercial research, contact [j.gale@ic.ac.uk](mailto:j.gale@ic.ac.uk). Other users contact Molecular Simulations Inc. More information at <http://www.ch.ic.ac.uk/gale/Research/gulp.html>.

Julian Gale, Imperial College, London

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## WinGX for Single-Crystals

The WinGX suite is a coherent collection of programs running under MS-Windows, in which the best available public domain software has been included. It includes industry standards such as SHELXS, DIRDIF, SIR92, SHELXL93 and ORTEP. Several absorption correction methods are available e.g. analytical, Gaussian grid, psi-scans, multi-scan, DIFABS, programs for the geometrical analysis results are provided, including PLATON, PLUTON, PARST and THMA11. CIF format is supported, checking of CIF-syntax and IUCr data validation is possible. The program itself and other associated programs are available from the following web-site: <http://www.chem.gla.ac.uk/~louis/software>.

Louis Farrugia, U. of Glasgow

## Beam Time Requests

A total of 644 applications were submitted for the September 1998 deadline for beam time between February and July 1999, for the 29 ESRF and 7 CRG beamlines that will be operating during this period. This is slightly lower than the number received in March 1998, the Block Allocation Group scheme accounting for a nominal drop by about 85 in the number of life sciences submissions.

## BCA/IUCr Congress Fund

The British Crystallographic Association has established a fund to be used to help organizers of future IUCr Congresses of Crystallography. Funds will be offered to the organizers of future IUCr Congress on the understanding that it will be repaid from any profits made by the Congress. It is strongly suggested that the money be used to fund the participation at the Congress of financially disadvantaged scientists. The British Crystallographic Association shall be acknowledged as a sponsor of the Congress in all literature. In the unlikely event of a loss being made by the Congress, no repayment will be due. Full details are available from the BCA.

## Crystallography Courses on the Web

An Advanced Certificate course in powder diffraction from the Dept of Crystallography, Birbeck College provides the necessary crystallographic and computational skills required for an understanding and usage of powder diffraction. The course, delivered via the Internet and making use of innovative technologies for distance learning is now accepting new registrations (<http://pd.cryst.bbk.ac.uk/pd/>). A course on *Protein Crystallography on the Web* is also being offered for students of biochemistry, molecular biology, bioinformatics, biophysics and/or organic chemistry who want to know in mainly non-mathematical detail how to determine protein structure, the quality of the structure, and how to interpret crystallographic papers. Course details are available at: <http://px.cryst.bbk.ac.uk/>



## Size/Strain Round Robin

The Commission on Powder Diffraction has installed a Round Robin on size and strain diffraction line-broadening effects to develop standards. An evaluation of different candidate materials could potentially lead to a certification procedure for a new NIST Standard Reference Material (SRM).

The Round Robin will have two phases: Methods of line-broadening analysis and broadening standards

**1st phase: Methods of line-broadening analysis** will include: 1. Stokes deconvolution + Warren-Averbach analysis, 2. Modified Williamson-Hall analysis, 3. "Double-Voigt" analysis, and 4. Rietveld-refinement analysis – modified TCH line-broadening model and Fourier series profile synthesis.

The "representative" diffraction patterns will be collected with Laboratory X-ray sources, Synchrotron X-ray sources and Neutron sources:

**2nd phase: Broadening standards** will include separate standards for size-dominant and strain-dominant broadening. The appropriate materials will be sent to the Round-Robin participants for the measurements.

If you wish to participate in either one or both phases, please fill out the form at the following addresses: <http://www.boulder.nist.gov/div853/balzar/> or <http://www.ccp14.ac.uk/ccp/web-mirrors/balzar/div853/balzar/> (CCP14 mirror).

## Lord Phillips of Ellesmere KBE, FRS. (1924-1999)

David Phillips was an outstanding scientist, one of the founding fathers of structural biology and an influential figure in science and government. He was Founder President of the British Crystallographic Association (1982-1984) and the spread of the Association's activities mirrored David's career in crystallography. He moved from intensity statistics and small molecule crystallography, to protein crystallography and instrument design. Protein crystallography led to proposals for structure/function relationships, homology modelling, fundamental understanding of thermal motion, and protein molecules of pharmaceutical interest. It is for his work with lysozyme that he will be most widely remembered. In 1966 he and the team working at the Royal Institution in London, solved the first structure of an enzyme, lysozyme and put forward proposals for its catalytic activity. The work opened the way to the explosion in the numbers of protein structures that are now being determined with modern technology and for the insights that these structures provide for the benefit of fundamental research, medicine and agriculture.

David was awarded a first class war-time degree in Physics, Mathematics and Electrical Communications (1942-1944; 1947-1948) at U. College Cardiff. The degree course was interrupted (1944-1947) for service in the RNVR. He remained at Cardiff for his Ph.D. and began work in crystallography under the supervision of A.J.C. Wilson. After a post doctoral period at the NRL, Ottawa (1951-1955), David came to the Royal Inst. of Great Britain in London in 1956 to join Uli Arndt in the design and construction of an automated diffractometer.

The solution of the 2 Å resolution structure of lysozyme in 1965 showed the complete path of the polypeptide chain folded into both alpha helices, that had previously been recognised in myoglobin, and beta sheet, a structure that had been predicted by Linus Pauling but not hitherto observed.

The inhibitor binding studies were extended to 2 Å resolution by early 1966. Data collection was laborious; a data set took 14 crystals and required nearly 3 weeks. A lysozyme-tri-N-acetylchitotriose complex led to a detailed interpretation of the lysozyme-inhibitor complex and the key elements of recognition at the catalytic site and a proposal for the way in which a hexasaccharide

substrate must bind. With C. Vernon's insights into mechanisms of glycoside hydrolysis, it was possible to make proposals for the catalytic mechanism. This was the first time that structure had provided an explanation of how an enzyme speeded up a chemical reaction. The extrapolation from inhibitor binding to the substrate binding was a remarkable leap of deductive reasoning, achieved in three days. David described these three days as the most rewarding that he had ever spent. David was awarded the Feldberg Prize, the CIBA Medal, the Royal Medal of the Royal Society, the Charles Leopold Meyer Prize of the French Academy of Sciences, the Wolf prize, the Aminoff medal of the Royal Swedish Academy of Sciences and many honorary doctorates.

In 1966, David was appointed Professor of Molecular Biophysics in Oxford U. In an article published in *Scientific American* (1966), Phillips showed how knowledge of the lysozyme structure could predict possible folding pathways that the protein might adopt as it was being synthesised on the ribosome. In another first, he, T. North and W. Browne used homology modelling to show how a protein distantly related in amino acid sequence (a-lactalbumin) might adopt the same structure as lysozyme. With graduate students (A. Bloomer, D. Banner, G. Petsko and I. Wilson) he solved the structure of glycolytic enzyme, triose phosphate isomerase, the first example of an 8-fold  $\alpha/\beta$  barrel protein.

David was elected to the Royal Society in 1967. From 1976-1983 he was Biological Secretary and Vice President at the Royal Society and was instrumental in introducing the Royal Society University Research Fellowships to promote the independent careers of gifted individuals. In his 1991 Bernal lecture, David put forward his view that scientific research must be organised so that "combined with the provision of the necessary infrastructure, it can release individual scientists to display their critically important gifts of spontaneity and originality". From 1983-1993 he was Chairman of the Advisory Board for the Research Councils (ABRC). His skills in committee were characterised by honesty,



Photo: W.L. Duax

and a gift for friendships.

His time at ABRC was not without controversy. On the one hand he needed to satisfy the increasing demands for funding from scientists faced with the growth of scientific opportunities, the need for more complex apparatus and facilities; the growing importance of interdisciplinary science, and the need for different organisations within which research can be conducted most effectively. On the other hand he fought to persuade Government to deliver more money while recognising the necessarily limited resources and pressures for concentration. He won the respect of both sides, emphasising that only the best science should be funded.

David was made Knight Bachelor in 1979, Knight Commander, Order of the British Empire (KBE) in 1989 and appointed in 1994 to a Life Peerage as Baron Phillips of Ellesmere (his birthplace). He joined the House of Lords Select Committee on Science and Technology and became Chairman in 1997 contributing to a report on Resistance to Antibiotics.

In the last years of his life he was ill with cancer but took a keen scientific interest in the treatment that held the disease at bay and he completed the final draft of a manuscript on how the lysozyme molecule was solved. He once listed among his interests "talking to children". He had a simplicity and directness that was equally effective with children and with the most august members of his committees. Many have commented on his great wisdom and on how they have benefited from his guidance and support. He was a special person who moved from academia to wider aspects of science policy, guided by a strong appreciation of history. He is much missed.

Louise N. Johnson  
*BCA Crystallography News*, June 1999



## Zdzislaw Galdecki (1924-2000)

Professor Marian Zdzislaw Galdecki, primary advocate of X-ray crystallography at the Technical University of Łódź, died of cancer at his home in Wrocław on January 29, 2000. He was 76. Though an excellent researcher, teacher and supervisor, he was most successful as a scientific manager. He was a Chairman of the Commission on X-ray Structural Analysis of Crystallography Committee of the Polish Academy of Sciences for many years and had the opportunity to employ his numerous talents. His enthusiastic support of the first Polish monocrystal diffractometer KM4 build by his colleagues, allowed Polish small molecule crystallography to flourish in 80's and 90's. He was also a Director of the National Centre Affiliate of the CCDC and a champion of the Cambridge Structural Database. He published over 200 research papers, several texts and chapters in monographs. He remained very active after retirement and worked to the last days of his life. He was honored by the Polish Ministry for his academic achievements eight times. His work with the pharmaceutical industry produced ten patents. Among his many students and five full professors, he had close ties with Hauptman-Woodward Medical Research Institute which resulted in thirty joint publications. He was always a very cheerful, enthusiastic and open minded person with a gift for finding similar research scientists.

M. Glowka



## Howard T. Evans (1920-2000)

Howard Tasker Evans Jr., 80, a scientist emeritus with the US Geological Survey and past president of the American Crystallographic Association, died Jan. 20 at his home in Rockville after a heart attack. Dr. Evans, an authority on the application of crystal chemistry to mineral systems, was a research chemist with the Geological Survey from 1952 to 1994. Since then, he had done research as scientist emeritus and also had served as a research associate with the mineral sciences division of the Smithsonian Institution. He served as a principal investigator for lunar sulfide minerals brought back from the moon in 1969. Over the years, he determined the crystal structure of more than 100 complex minerals. Dr. Evans was a 1985 recipient of an Interior Department Meritorious Service Award and had served as a fellow, councilor and associate editor with the Mineralogical Society of America. He also helped organize and lead the Washington Crystal Colloquium. He served as a special advisor to the International Atomic Energy Commission for an X-ray diffraction laboratory. He was the author of more than 150 technical publications and took part in early research that resulted in a Nobel Prize in chemistry for Jerome Karle and Herbert Hauptman in 1985. Dr. Evans was born in the Panama Canal Zone and raised in Wellesley, Mass. He was a 1942 chemistry graduate of the Massachusetts Institute of Technology, where he also received a doctorate in inorganic chemistry. Be-

fore coming to Washington and joining the government, he taught and performed research at MIT and was a research physicist with Phillips Laboratories in Westchester, NY.

From the Washington Post

## Shizuo Miyake (1911-1999)

Professor Shizuo graduated from the U. of Tokyo, and started research predominantly on X-ray and electron diffraction, working for S. Nishikawa. In the late 1950's he was appointed to a professorship at Tokyo Inst. of Technology, and soon moved to the U. of Tokyo, Inst. of Solid State Physics. Until his retirement he was the Director of that Institute.

He published numerous research papers in his own name, or in collaboration with others, particularly his students. The most famous ones include: "an experimental discovery of a failure of Friedel's law ( $|F_{hkl}| = |F_{\bar{h}\bar{k}\bar{l}}|$ ) in electron diffraction.

He attended the IUCr Congress and General Assembly several times, initially in 1954, and often as the head of the Japanese delegates. He also served IUCr as a co-editor of *Acta Crystallographica* and a commission member. Indeed, Professor Shizuo Miyake had been one of the leading figures in Japanese Crystallography for a long time.

Yuji Ohashi

### 9<sup>th</sup> Slovenian-Croatian Meeting

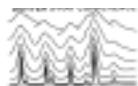
SLO-CRO-9 will be held **June 15-17, 2000** in Gozd-Martuljek in the Julian Alps, Slovenia. All aspects of crystallography and its application will be covered. Contributed oral papers only and will be published in the Book of Abstracts. No registration fee. The official language of the meeting is English. Plenary lecturers: C. Giacovazzo (Bari), Ch. Baerlocher (Zurich), A. Tonejc (Zagreb) and I. Turel (Ljubljana).

Contact: I. Leban, Chemistry, Uni, PO Box 537, 1001 Ljubljana, Slovenia. Tel: 386 61 1760 582; Fax: 386 61 1258 220. e-mail: [ivan.leban@uni-lj.si](mailto:ivan.leban@uni-lj.si); <http://rcul.uni-lj.si/~fn01leban/slocro.html>.

### Supramolecular Japan

The 11th Int'l Symposium on Supramolecular Chemistry (ISSC XI) will be held in Fukuoka, Japan **July 30-August 4, 2000**. Topics will include: Molecular Recognition, Inclusion and Clathrate, Self-Assembly, Molecular Organization and Alignment Control, Molecular Network, Liquid Crystal and Crystal Engineering, Supramolecular Function, Biological Supramolecular System and Model, Physical/Analytical Aspect, Sensing, Templated Reaction and Catalysis, Supramolecular Chirality, Photo- and Electrochemical Response, Probe Microscopy, Molecular Device and Molecular Machine, Nanomaterial and Nanotechnology, Bioorganic and Bioinorganic Aspect, Gene-, Protein-, and Glycoscience and Technology, etc.

Abstract deadline is April 30, 2000. For further information contact <http://www.issc.kyushu-u.ac.jp>. Symposium chairman is Y. Aoyama.



### 2000 Denver X-ray

The 2000 Denver X-ray Conference will be held **July 31 - August 4** in Denver, Colorado, USA. Detailed conference information and a tentative program is available at <http://www.dxcicdd.com> or contact D. Flaherty, Conf. Coordinator, ICDD, 12 Campus Blvd., Newtown Square, PA 19073-3273, FAX: 610-325-9823, [flaherty@icdd.com](mailto:flaherty@icdd.com).



### Indaba III

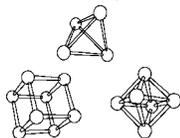
A Workshop on Symmetry and Structure: Symmetry Breaking, Chirality and Disorder in Molecules and Crystals will be held **August 6-11, 2000** at Skukuza, Kruger National Park, South Africa. It is being presented by the South African Crystallographic Society under the auspices of the International Union of Crystallography Commission on Structural Chemistry sponsored by the IUCr.

Abstracts must be received no later than March 20, 2000. For information, visit the website at [hobbes.gh.wits.ac.za/indaba](http://hobbes.gh.wits.ac.za/indaba).

### ECM19

The 19th European Crystallographic Meeting (ECM19) will be held in Nancy (300 kms east of Paris, France) **August 25-31, 2000**. All fields related to crystallography will be discussed, from mineralogy to biomolecular sciences, including physics, chemistry, material science, theoretical methods and instrumentation.

Further information is available at <http://www.lcm3b.u-nancy.fr/ecm19/>.



### IWPCPS-1

First Int'l Workshop on Physical Characterization of Pharmaceutical Solids (IWPCPS-1) **September 24-29, 2000** in Lancaster, PA, USA. A unique workshop designed for scientists in the areas of drug discovery, preformulation, formulation, stability testing, product development, product quality control and analytical services.

For information contact: A. Zakrzewski, FAX: 610594 2082, [Angeline@ASSCI.com](mailto:Angeline@ASSCI.com); [www.assci.com/~marekz/IWPCPS-1.htm](http://www.assci.com/~marekz/IWPCPS-1.htm).

### X-rays in Research and Industry

The Malaysian Inst. for Nuclear Research (MINT), in cooperation with U. Sains Malaysia, U. Malaya, SIRIM Bhd, and the Malaysian Nuclear Society (MNS), is jointly organizing the 2nd Asian Conference on X-Rays and Related Techniques in Research and Industry (ACXRI 2000) in Kuala Lumpur, Malaysia, **November 20-22, 2000**. For information contact [meor@mint.gov.gov.my](mailto:meor@mint.gov.gov.my).

Nahrul Khair Alang Md. Rashid, Conf. Chair

### Erice 2001

The 32nd crystallographic event at Erice, Italy, "Strength from Weakness: Structural Consequences of Weak Interactions in Molecules, Supermolecules, and Crystals" will take place **May 23-June 3, 2000**.

This Course will demonstrate the significance and applicability of small structural differences, including their role in molecular recognition, following a discussion in the demands and caveats of their determination. Special attention will be paid to the advantages and limitations of each technique of structure determination, and to the concerted use of different techniques, both experimental and computational.

The Course is highly interdisciplinary as it involves all experimental and computational techniques currently used to determine the structure of molecules. It will bring together scientists from a number of different fields, such as X-ray crystallography, neutron crystallography, gas-phase electron diffraction, microwave spectroscopy, high resolution vibration-rotation spectroscopy, NMR spectroscopy, computational and theoretical chemistry, as well as research workers of broad areas who are primarily the users of structural information. There will be in-depth discussions on all facets of the determination of small structural differences caused by weak interactions, and of their chemical relevance. Junior research workers will especially benefit from this opportunity.

To date the following lecturers have agreed to participate: J. Bernstein (Ben Gurion U., Israel), R. S. Berry (U. of Chicago, USA), J. Demaison (U. of Lille, France), G.R. Desiraju (U. of Hyderabad, India), A. Domenicano (U. of L'Aquila, Italy), G. Gilli (U. of Ferrara, Italy), I. Hargittai (Budapest Tech U., Hungary), M. Hargittai (Hungarian Acad of Sciences, Budapest, Hungary), T. M. Klapoetke (Ludwig-Maximilians U., Germany), J. Leszczynski (Jackson State U., USA), H. Moellendal (U. of Oslo, Norway), U. Roethlisberger (ETH, Zurich, Switzerland), D.R. Salahub (NRC, Ottawa, Canada), P. Schwerdtfeger (U. of Auckland, New Zealand).

For information contact P. Spadon, FAX: 39 049 8275239, [paola@pdchor.unipd.it](mailto:paola@pdchor.unipd.it), [www.geomin.unibo.it/orgv/erice/accurate.htm](http://www.geomin.unibo.it/orgv/erice/accurate.htm).

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## Contributors

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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.

## MAY 2000

- 14-19 ♦ **8th Int'l Conf. on Crystallization of Biological Macromolecules.** Sandestin, FL, USA. <http://ICCBM8.cmc.uab.edu/>.  
 25-4 ♦ **Methods in Macromolecular Crystallography, 30th Course** (A NATO Advanced Study Institute). Erice, Italy. Contact: [www.geomin.unibo.it/orgv/erice/johnson.htm](http://www.geomin.unibo.it/orgv/erice/johnson.htm).  
 25-4 ♦ **Prospectives in Crystallography of Molecular Biology, 31st Course.** Erice, Italy. [www.geomin.unibo.it/orgv/erice/johnson.htm](http://www.geomin.unibo.it/orgv/erice/johnson.htm).

## JUNE 2000

- 14-17 ♦ **The Sixth European Symposium on Calcium Binding Proteins in Normal and Transformed Cells.** Paris, France. F. Russo-Marie, M. Bajole, ICGM, FAX: 33 0 1-40-51-77-49, [u332-russo@cochin.inserm.fr](mailto:u332-russo@cochin.inserm.fr), [www.cochin.inserm.fr/eCs](http://www.cochin.inserm.fr/eCs).  
 15-17 ♦ **9th Slovenian-Croatian Meeting (SLO-CRO-9).** Gozd-Martuljek in the Julian Alps, Slovenia. See Page 31.

## JULY 2000

- 22-27 ♦ **American Crystallographic Assn Annual Meeting (ACA '00).** St. Paul, MN, USA. [www.hwi.buffalo.edu/ACA](http://www.hwi.buffalo.edu/ACA).  
 25-29 ♦ **Aperiodic 2000.** Nijmegen, The Netherlands. [www.sci.kun.nl/tvs/aperiodic/](http://www.sci.kun.nl/tvs/aperiodic/)  
 31-4 ♦ **2000 Denver X-ray Conference.** Denver, Colorado, USA. See Page 31.

## AUGUST 2000

- 6-11 ♦ **Indaba III: Symmetry Breaking, Chirality and Disorder of Molecules and Crystals.** Skukuza, Kruger Nat'l Park, South Africa. See Page 31.  
 25-31 ♦ **European Crystallographic Meeting (ECM19).** Nancy, France. See Page 31.

## SEPTEMBER 2000

- 3-8 ♦ **Solid State Chemistry 2000.** Prague, Czech Republic. [www.iic.cas.cz/ssc2k.htm](http://www.iic.cas.cz/ssc2k.htm).  
 24-29 ♦ **First Int'l Workshop on Physical Characterization of Pharmaceutical Solids (IWPCPS-1).** Lancaster, PA, USA. See Page 31.

## NOVEMBER 2000

- 20-22 ♦ **2nd Asian Conference on X-Rays and Related Techniques in Research and Industry (ACXRI 2000).** Kuala Lumpur, Malaysia. See Page 31.

## MAY 2001

- 23-3 ♦ **Strength from Weakness: Structural Consequences of Weak Interactions in Molecules, Supermolecules, and Crystals.** Erice, Italy. See Page 31.

## Deadlines

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