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INTERNATIONAL UNION OF Crystallography

NEWSLETTER

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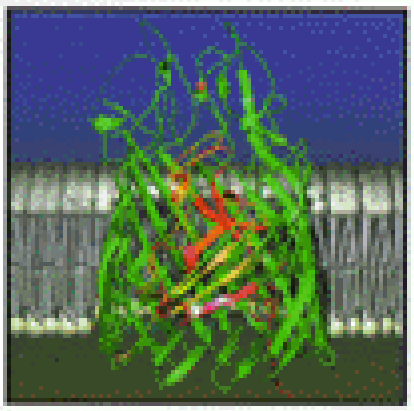
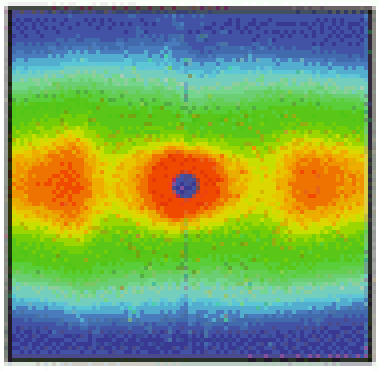
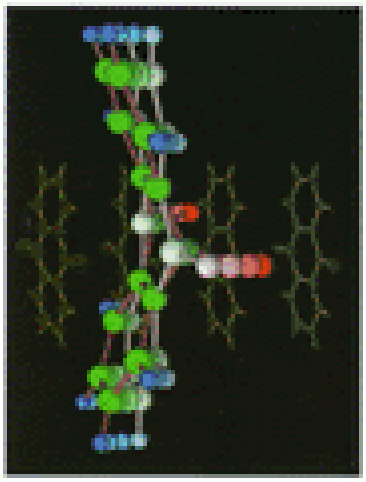
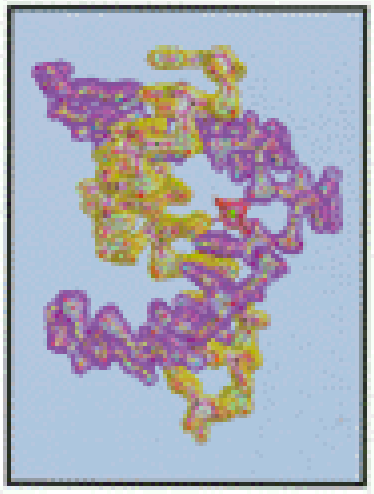
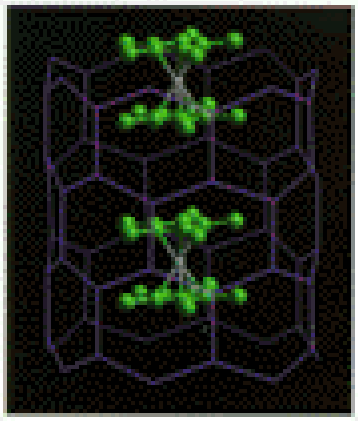


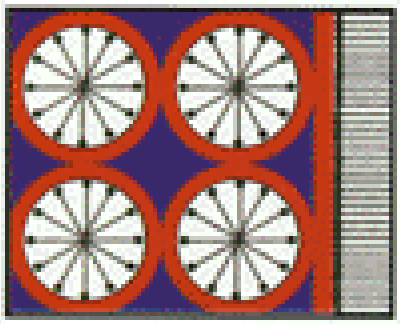


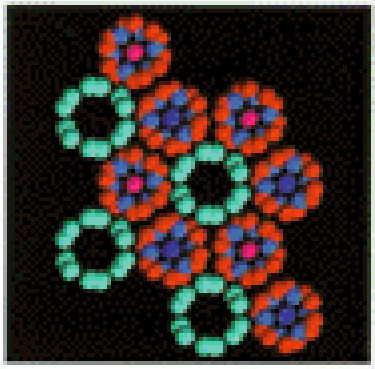


IUCr XVIII
Glasgow 1999









Ted Baker

Of Mentors and Role Models

As the next Congress and General Assembly of the IUCr approaches it is worthwhile to think for a moment about the importance of mentors and role models in science. The public perception of scientists is often of cool, analytical minds heading logically towards a goal. In fact, of course, scientific research is an intensely human activity involving emotion, excitement (and sometimes despair), rivalry and cooperation. In this climate, it is essential that there be role models and mentors who can provide support, advice, the appropriate ethical standards, and above all time, for young scientists.

I have been extraordinarily lucky in my own scientific career, with graduate supervisors (Neil Waters and David Hall) who enabled me to learn how to approach research and steered me in the right directions, and postdoctoral mentors, David Phillips and Dorothy Hodgkin, who provided wisdom, inspiration and friendship. Dorothy it was who inspired me with the courage to return to my own country to build up a programme of macromolecular crystallography from scratch. And all along there have been wonderful friendships made with people whom I admire and respect, from many different countries.

The point of these comments is that young scientists, both men and women, need support and encouragement. The IUCr offers financial help to enable young crystallographers to attend scientific meetings, and I regard this as one of our most important activities. It is only part of what is needed, however. The Glasgow Congress will also be a great opportunity for well established crystallographers to take the time to talk with students, postdocs and other young scientists from round the world, to listen to them and to their aspirations, and to discuss their science. Likewise it is an opportunity for young crystallographers to seek out those whose names they may only know from the literature, to discover that they are real people, and perhaps to begin a lifetime's association and friendship. I look forward to seeing you all in Glasgow.

Edward N. Baker
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The IUCr Newsletter is distributed to 587 libraries and 15,000 crystallographers and other interested individuals in 39 countries. Feature articles, meeting announcements and reports, information on research or other items of potential interest to crystallographers should be submitted to the editor at any time. Submission of text by electronic mail and graphics, slides or photographs by express mail is requested. Items will be selected for publication on the basis of suitability, content, style, timeliness and appeal. The editor reserves the right to edit. Cost of distribution in Australia, 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.

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Matters pertaining to Advertisements should be addressed to W.L. Duax or P. Coley at the above address. In Japan, contact Prof. Yukio Mitsui, Dept. of BioEngineering, Nagaoka U. of Technology, Nogaoka, Niigata 940-21, Japan, FAX: 81-258-47-9400.

On the Cover: The full range of crystallographic research to be presented at the XVIII Congress of the International Union in Glasgow, August 4-13, 1999, is reflected in illustrations generously provided by (clockwise from upper left) Hans Deisenhofer, Nobuo Niimura, Hans-Beat Bürgi, John McKay, Janusz Lipkowski, John White, Lynne B. McCusker, and Ken Holmes. Composite by Patricia Coley. See page 21.

Contributors: N.M. Allinson, H. Berman, P. Bourne, I.D. Brown, E. Dodson, V. Evsyunin, R.B. Ferguson, G. Gilliland, A. Hamilton, J. Hauser, A. Hunter, A. Kashaev, W. Melik-Adamyam, A. Mishnev, R. Nelmes, G. Newton, J. Parise, V. Pattabhi, D. Poleti, J. Pons, A. Revenko, and T. Safonova.

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Letters to the Editor

Dear Bill:

It was a pleasure to receive the current issue (Vol. 7, No. 1) of the IUCr Newsletter. I was particularly pleased to see the item on Crystallographic Nomenclature.

The coverage of last year's meetings of IUCr affiliates was surely a worthy and interesting use of your limited space. Future meeting reports such as these would be more useful to many readers if each were accompanied by access to a website with detailed information. Although several URL's are indeed printed in this issue's reports, the information could be enhanced. A first step would be to provide all available abstracts of papers presented on the website, with the appropriate URL given in the meeting report; as meeting organizers increasingly require abstracts to be submitted electronically, this will become easy to do. A second step would be for the organizers to post an expanded version of the report submitted to the Newsletter, since the limitations of printed space will not apply. No doubt there are many further steps that should be considered!

Sidney C. Abrahams, Southern Oregon U.

Dear Sidney,

Thanks for your comments and suggestions. When websites containing meeting abstracts are available, we will cite them in future reports. Less than half the session chairs at the AsCA, ACA, or ECM meetings provide reports. Some of the reports were abbreviated in the newsletter and in the future we will try to post the originals on the Newsletter web site and note that.

Bill

Dear Bill,

It was very kind of you to send me the color picture and the issue of the IUCr Newsletter. I was touched by the fact that the memorial for Ken was held. You may be interested to know that I have been in touch with the chief archivist at UCLA and I'm in the process of collecting Ken's papers to be kept at the University. Also, the large lecture hall where Ken gave many classes has been named with a bronze plaque and title above the large double doors - The Kenneth N. Trueblood Lecture Hall.

Jean Trueblood, Los Angeles, CA

Dear Jean,

I am sure that many crystallographers around the world will be pleased to know of UCLA's plans to honor Ken.

Bill

Dear Bill,

I always appreciate your excellent photographs which appear in the IUCr's prestigious organ. I happened to notice one in the ECM-18 report where the participants were described as being 'in Phase and ready for Transition'. This is true to the extent that our minds were in phase with the science and, poised for your photograph, we were ready for synchronous transition to lunch. Incidentally, the caption strongly implies an association with the microsymposium on Phase Transitions when, in fact, we were at the parallel session on Neutron Scattering. Am I still coherent?

Jon Cooper, U. of Southampton

What's Hot and What's Not?

This issue contains the last of the reports filed by the session chairs at ECM-18. These reports were submitted in a timely fashion, but could not be included in the last issue due to space limitation. Also included in this issue is a description of the martensitic effect. A microsymposium was devoted to this topic at the ECM 18 in Prague. Jaume Pons kindly agreed to prepare a one page article on the effect in terms that could be easily understood by the average crystallographer. I found the phenomenon fascinating and his description to be lucid and informative. I welcome similar brief articles on other aspects of crystallographic theory, techniques or applications for inclusion in future issues.

Sidney Abrahams in a letter to the editor (page 2) expresses concern that the meeting reports in the IUCr Newsletter are incomplete and notes that in the age of www, it should be possible to place all abstracts and all meeting reports on the web in a timely fashion.

In an aside in his remarkable chapter in Reviews of Crystallography, Vol. 7, 1998, entitled "The Crystal Packing of Organic Molecules: Challenge and Fascination Below 1000Da" Angelo Gavazotti expresses the same concerns that meeting reports in the newsletter are incomplete. Gavazotti goes further and suggests that there is a bias in reporting, favoring macromolecular crystallography. Gavazotti's entertaining, thought provoking, and provocative chapter is well worth reading, with something to offend almost everyone (or so he hopes). Gavazotti chides the IUCr Newsletter editor for relegating non-macromolecular reports to "future issues of the newsletter" that never reach Italy.

Gavazotti seems to call for a holy war against macromolecular crystallography. I don't believe the promotion of discord between different parts of the crystallographic community is in the best interest of the discipline. The beauty of crystallography is that it provides reliable information about all kinds of materials. It is often the most reliable and detailed information that can be obtained. Editing material for the newsletter challenges me to think about many of those applications and I never fail to be enlightened and informed by the wide range of applications of crystallography and to see areas of cross disciplinary overlap among them. I like to think I gain from considering crystallographic applications outside of my own research field.

The ACA meetings are heavily weighted toward macromolecular crystallography due to economics. The Powder diffraction community seems to be drawing away from the larger community to discuss formation of an international powder society. Coverage of mineralogical crystallography is meager at most national and international crystallographic meetings. Small, cozy specialist meetings have great appeal, but they can be insular, elitist and just a trifle smug. In my estimation, the IUCr Congress is the only venue that brings all aspects of crystallography together. In my opinion, you can't have too many crystallographers or too many in one place.

Uniform handling of abstracts and early posting to the web is becoming common practice. Beginning with the 1995 meeting in Montreal, the ACA has placed all abstracts on the web well before the meeting. Some meeting participants request that their abstract not be released to the web until the opening of the meeting. Unfortunately, meeting reports require additional effort from session chairs. An extended final report on ECM-18, including all abstracts can be read at http://krystal.karlov.mff.cuni.cz/ecm/. The ACA meeting reports that appear in the last issue were condensed from a long report in the *ACA Newsletter* (Fall, 1998). The ECM and AsCA reports were prepared from reports of the chairs of sessions and plenary lectures. At ECM there were 60 microsymposia and 10 plenary lectures and 22 reports were submitted. At the AsCA meeting there were 15 microsymposia and 4 plenary lectures and 6 reports were submitted.

Choose your session chairs carefully if you want to have your area of crystallography well represented in meeting reports.

William L. Duax, Editor

Good Homes Required for Crystallographic Equipment

Dr M. Moore (Royal Holloway, U. of London) would be pleased to hear from anyone who would like to make offers for a Weissenberg camera, powder diffractometers, powder cameras, an X-ray generator and other items. In good condition. One careful owner. Further details on request. e-mail: M.Moore@rhbnc.ac.uk, Fax: 01784-472794.

18th International Union of Crystallography Congress

As the Millennium draws to a close, August sees the United Kingdom playing host to the 18th IUCr Congress, which is expected to be the biggest yet with over 2500 delegates attending. The host city for the congress is Scotland's other great city, Glasgow, renowned for its hospitality and liveliness as well as boasting a wealth of cultural amenities and awards, including the title of UK City of Architecture and Design 1999. Running from 4th August until 13th, the Congress will take place at the Scottish Exhibition and Conference Centre (SECC), one of the most modern and attractive conference centres in Europe and conveniently located in the heart of Glasgow yet only 20 minutes from the International Airport. The Congress will present new and exciting advances in all areas of crystallography and will serve to highlight the crucial role played by crystallography in pushing back scientific frontiers across a wide spectrum of scientific disciplines.

The Congress lecture programme is split into 5 broad brush categories covering chemical, biological, theoretical/fundamental, materials and industrial applications of crystallography, with considerable overlap between these categories. This year however, industrial crystallography and its applications takes on a more prominent role with 14 'Industrial' micro-symposia being incorporated into the main body of the Congress(between 4th and 10th August) instead of satellite meetings as in previous years.

The programme schedule operates a 'sandwich' type structure. There will be two keynote lectures running in parallel both at the beginning and at the end of each day with the filling consisting of two sessions of six parallel microsymposia – one session in the morning and one in the afternoon. The middle of the day will be given over to the poster sessions and lunch, which can be enjoyed simultaneously in the main Exhibition Hall. All in all, delegates can look forward to 32 keynote lectures, 96 microsymposia and over 1,700 poster presentations during the nine day Congress. Would be astronomers have not been forgotten either. The programme will be suspended from 11-11.30am on the morning of 11th August to allow delegates to enjoy (Scottish weather permitting!) the 82% eclipse of the sun, which takes place at 11.16 that morning.

The opening speech of the Congress on the evening of the 4th will be given by Prof. Aaron Klug, president of the Royal Society, who will also chair the first plenary session. The scientific programme commences the following day. The keynote speakers will deliver lectures right across the spectrum of crystallographic science. Space constraints prevent a full listing here, but some of the highlights will include (in alphabetical order):

•Elena Boldyreva (Inst. of Solid State Chemistry, Novosibirsk, Russia) – "Solid State Reactions" – Thursday 5th, p.m.

•Jennifer Doudna (U. of Yale, USA) – "Crystal Structures of Ribosymes" – Wednesday 11th, p.m.

•Jack Dunitz (ETH, Zurich) – The Bragg Lecture: "Polymorphism – The Same yet Different" – Saturday 7th, a.m.

•Michele Parrinello (Max Planck Inst., Stuttgart, Germany) – "Role and Perspectives of ab initio Molecular Dynamics in Crystallography" – Thursday 12th, a.m.

•Jim Scott (U. of NSW, Australia) – "Crystallographic Aspects of Ferroelectric Memories" – Thursday 5th, a.m.

•Paul Sigler(U. of Yale, USA) – "Chaperonin Assisted Protein Folding: The Final Step in Genetic Expression" – Saturday 7th, p.m.

•Josh Thomas (U. of Uppsala, Sweden) – "Crystallography and the Lithium Ion Battery" – Sunday 8th, a.m.

•Richard Welberry (ANU Canberra, Australia) – The Lonsdale Lecture: "Diffuse Scattering" – Saturday 7th, p.m.

The Microsymposia subject areas and array of presenting speakers are no less diverse, giving delegates a huge choice of topics. Titles range from: "Viruses and Viral Protein", "Drug Discovery and Design" and "Hot Macromolecular Structures" in the biological areas to "New Frontiers in High Pressure Crystallography", "Molecular Magnets" and "Nanomaterials" in the field of Industrial and Materials Crystallography. A special emphasis has been placed on the interaction between crystallography and both materials and biological sciences, which will be reflected in the subject content. For example, developments in the role of 'bio-informatics' (where chemical and crystallographic data bases can be harnessed in a wide variety of molecular modelling and interaction applications) will be highlighted. Similarly, exciting developments in high pressure and low temperature crystallography will be presented.

As in previous Congresses, Glasgow 1999 offers delegates the opportunity to display posters of their current research activities. With the deadline for entries now closed, the organisers confirm that over 2,300 abstracts have been received with a record number of poster presentations scheduled for the meeting. Contributions have been received from all corners of the globe, from Bangladesh to Brazil, Chile to China and New Zealand to the Netherlands. Some of the more intriguing poster abstract titles include: "Turkish Ornaments are Twins of Crystals", The Crystal Structure of Adenovirus Knob bound to its Cellular Receptor Car" and "Wood Fibre Diffraction using CCD Detectors in Forest Planting Programs"!

The Congress also incorporates a large commercial exhibition with many of the major companies involved in the production and use of crystallographic software and hardware exhibiting their products and services. Running from 5th – 9th of August, the exhibition will feature all the big names in crystallographic technology and instrumentation and will also provide space for a poster area, general seating, eating facilities and an Internet Café from which delegates can read their e-mail. All in all, it should provide a lively and stimulating environment in which to discuss crystallography.

As well as the lecture and poster presentation programme, a number of Open Commission Meetings are scheduled to take place throughout the Congress, paralleling either a microsymposia or poster session. There are also three workshops, which take place on 4th August covering "Structure Factor Phase Determination", "The Cambridge Structural Database" and "Structure Solution from Powder Diffraction Data". For those with some extra time at the beginning or end of the Congress, there

are three satellite meetings on "Synchrotron Radiation", "Structural and Dynamical Aspects of Molecular and Ionic Solids Using Neutrons" and "CCDC Databases"*. These will be held at Daresbury, Oxford and Cambridge respectively.

Because 'all work and no play makes Jack a dull boy', the organisers have not forgotten the social programme! The opening ceremony will be accompanied by a Scottish Pipe band of the 51st Highland Division complete with singers and dancers and this ceremony will be followed up with a number of events throughout the Congress. These include both whisky (what else?) blending and whisky tasting evenings, a delegate reception in the Kelvingrove Art Gallery and Museum and for those with more energy a 'Learn to Dance' session that aims to hone the Scottish Dancing skills for the Gala Ceilidh, which takes place the following evening. For those new to the shores of Scotland, a number of tours are also available taking in areas such as Loch Lomond, The Trossachs and the Isle of Arran and offering some of the finest mountain scenery in Europe.

Registration for the IUCr XVIIIth Congress is available right up until the start, although delegates who register before 1st June 1999 will receive a £50 reduction in their registration fee. For details on how to register, contact: Crystallography Congress 1999, Northern Networking, Congress Central Office, 813 South St, Glasgow G14 0BX, Tel: +44 (0) 141 954 4441, Fax: +44 (0) 141 954 2656

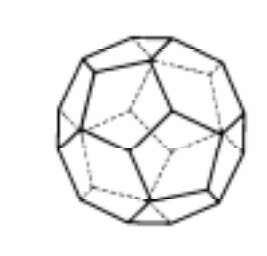
The last IUCr Congress of the Millennium promises to be the most successful ever. The organisers look forward to seeing you there and feel certain that all the attending delegates will find the meeting a most rewarding experience.

Acknowledgements

A lot of hard work has gone on behind the scenes to ensure the Glasgow 1999 Congress is a great success. Thanks must go to the 'Abstracts Team' at the Rutherford Lab for a truly amazing job of receiving and registering and coding over 2,300 abstracts ready for incorporation into the abstracts book. This is the first time that Congress abstracts have been dealt with solely by electronic submission and the operation's success is in no small part due to their efforts. Also thanks to the part-time 'Programme Team' at Durham directed by (the tireless!) Professor Judith Howard for gathering together the information on the 600+ speakers and also assisting the Bursary Committee in assigning awards to attending students. Finally thanks to the 'Local Team' headed by Chris Gilmore and helped by 'Northern Networking' in organising registrations, accommodation and the social programme which will help to make Glasgow 1999 a really memorable experience.

Andrew Hamilton BSc Hons GRSC

**Ed. Note: Just prior to press time, the CCDC satellite was cancelled.*



Offer of Several 1960's Volumes of the French Journal of Crystallographic Abstracts *Structure De La Matiere*

I offer to any interested individual, library, etc., for the cost of shipping, about seven years' volumes (approx. 75 numbers) of this journal which was included with membership in the American Crystallographic Assn during the 1960's.

This journal was published (in French) by the Centre National De La Recherche Scientifique in Paris with the full title/subtitle

Bulletin Signaletique 6, Structure De La Matiere
Crystallographie - Solides - Fluides - Atomes - Ions - Molecules

The volumes and numbers I have available are: Vol XXII, 1961, nos. 3-10 and TABLES [= index], Vols. XXIII - XXVIII, 1962-1967, nos. 1-11/12, TABLES (complete), Vol. XXIX, 1968, nos. 1-3.

Anyone interested in further details including the cost of shipping (total weight approx. 35 kgs.) which I would be willing to explore, contact me: Dept. of Geological Sciences, U. of Manitoba Winnipeg, Manitoba R3T 2N2 Canada, Tel. 204 474 1731, FAX 204 474 7623, ferguson@ms.umanitoba.ca.

Robert B. Ferguson

High Pressure Commission Workshop

The High Pressure Commission of the IUCr held an international workshop at the Argonne National Laboratory, Nov. 14-17, 1998, entitled "Synchrotron, Neutron and Laboratory Source Crystallography at High Pressure". This was the first of the Commission's activities since it was formed at the Seattle Congress in 1996. The formal sessions were illustrative of the full range of crystallography using high-pressure techniques. The IUCr, The Center for High Pressure Research (CHiPR), GeoSoilEnviro-Consortium for Advanced Radiation Sources (GSECARS) and the Advanced Photon Source (APS) provided financial support for the meeting. Most of the program responsibilities were borne by the Commission, with John Parise acting as chair of the local and program committees, working closely with Commission chair, Richard Nelmes. We would like to acknowledge the assistance of N. Lazarz (Sectors Coordinator for GSECARS at the APS, Y. Wang, M. Rivers, D. Franklin, J. Brunsvold (ANL Conference Services) and other GSECARS staff.

The oral sessions and over 75 poster presentations emphasized the very latest science and techniques. The meeting attracted 117 participants representing 59 institutions and 14 countries, including 23 young scientists, 17 of whom received support from IUCr funds. A number of the poster presenters gave a 3 minute introduction to their work in a special session on facilities and techniques. Several other invited "poster orals" were added to the oral program.

The first session highlighted recent developments in "soft matter". This sub-discipline, being covered in a forum of the High-Pressure Commission for the first time, was introduced by a talk from S. Gruner, who outlined the potential for using the large effects observed with modest application of pressure and concluded with a summary of the technical challenges. The session included stimulating presentations on pressure-induced unfolding of proteins (G. Hummer), phase behavior of mesophases and proteins (R. Winter), and packing of alkanes under pressure (H. King). Poster orals covered the structure of melamine (P. Dera) and the high-pressure behavior of gelatin (W. Poon).

Elasticity and rheology are areas important to members of the Earth and materials community. Recent developments in theory and in the design of apparatus at synchrotron beamlines has allowed interpretation of changes in powder diffraction patterns in terms of relaxation and stress-strain behaviors induced by heating at high pressures. T. Duffy and A. Kavner presented their latest results on the determination of lattice strains and P/T calibrations in the diamond anvil cell. Unfortunately, a bar on Indian scientists entering a DoE facility prevented A. Singh from attending.

On Saturday evening J. Jorgensen traced the history of "Thirty Years of Neutron Diffraction at High Pressure" which, in large part, began and flourished at the Argonne National Lab.

The two sessions on technical developments covered the latest in optimizing the diffraction experiment for precision (M. Kunz and R. Angel), unit-cell indexing and structure solution from complex powder data (S. Belmonte), and the use of maximum entropy techniques to extract information from a powder diffraction experiment (M. Takata). Poster orals dealt with the accurate determination of the pressure scale (D. Weidner) and development of drilled diamonds to permit the use of low energy x-rays (C. Colle). This latter development complements recent progress in the use of beryllium gaskets by the group at the Geophysical Laboratory. Y. Katayama presented new developments in studies of liquids at high P and T, and G. Fiquet presented technical developments that are taking studies of earth materials close to the conditions of the Earth's lower mantle and core.

Theoretical presentations, by R. Cohen and S. Scandolo, emphasized transitions and behavior under extreme conditions important to the Earth and other planetary interiors. S. Saxena presented some corresponding experimental results obtained from both synchrotron and laboratory-based sources employing imaging plate and CCD detectors. Twenty invited oral presentations of posters on facilities and techniques followed a talk by G. Shen concerning developments of the APS.

Sessions were devoted to magnetism, superconductivity, general bonding and materials characteristics as a function of pressure. The first of these included presentations on spin-Peierls transitions (M. Nishi), neutron diffraction magnetic studies to 50 GPa (I. Goncharenko), studies of GMR manganites (D. Argyriou), superconductivity (D. Sheptyakov) and a comparison of the effects of applied vs. chemical pressure in magnetic studies (I. Mirebeau). A session emphasizing structure, bonding and materials featured talks by P. McMillan on twinning and packing of boron-rich clusters, H. Fujihisa on the structures of HCl and HBr, K. Syassen on the new structures of Cs-V and Si-VI, K. Kusaba on phase

Participants at the Workshop "Synchrotron, Neutron and Laboratory Source Crystallography at High Pressure". Photo curtesy of John Parise.

equilibrium of group II-VI semiconductors at high P and T, and D. Haüsermann on the latest results from the very active group at beamline ID30 at the ESRF, including work on semiconductor phase diagrams in a Paris-Edinburgh large-volume cell. M. McMahon complemented this session with an invited poster oral on new structures and transitions in GaAs.

The final day featured spirited sessions on ices and hydrogen bonding, and spectroscopic studies. W. Kuhs provided an overview of ices and ice clathrates at lower pressures, followed by talks dealing with phase transitions and structures of liquid water and amorphous (glassy) and crystalline ice (D. Klug and M.-C. Bellissent-Funel). J. Loveday presented results of the Paris-Edinburgh collaboration on neutron diffraction study of ices up to 25GPa, and R. Hemley on studies of ice to megabar pressures and D. Marx on complementary *ab initio* calculations of protons in ice in that range.

The final session of the meeting, "spectroscopic studies at high pressure", covered the latest developments in what is/will be possible in 1999. S. Klotz presented work much extending the pressure range of inelastic neutron scattering. M. Pasternak spoke of his Mössbauer spectroscopy on FeO and advanced pressure cells for studies beyond 100GPa. W. Bassett and R. Mayanovic gave closely-related talks dealing with the design of a special DAC to allow EXAFS studies at low-energy edges. They presented results on zinc (II) complexes in hydrothermal fluids. The meeting was given a splendid finale with a talk from H. Mao on recent developments in X-ray spectroscopy and the many exciting prospects of the new beamline concept at the APS (the High Pressure Collaborative Access Team or HP-CAT).

Carol Brock and an old friend from Kentucky attending the AsCA meeting in Malaysia. (Photo WLD)

Tours of the APS and IPNS facilities, were conducted in parallel with posters one afternoon. The highlight of the banquet was a presentation by Malcolm McMahon of essential linguistic guidelines for those attending the Glasgow Congress. In bare knees and a tartan car-rug, he assailed the crowd with some of the finest Scots humor heard since Sean Connery played that Russian submarine commander!

The participants plan to meet again in Glasgow where six oral sessions will continue to develop many of the topics of this landmark meeting.

John Parise and Richard Nelmes

Crystal Simulation Workshop

A workshop on Simulating Crystals as a Teaching Tool and Analyzing Defect Structures will be held during the IUCR Meeting in Glasgow, Aug. 11, 1998, under the auspices of the German Crystallographic Assn.

Simulating crystals in a computer is an efficient tool to teach crystallography and diffraction physics. Clusters of atoms and crystal structures, free from constraints imposed by real materials can be used to explain and explore different features of diffraction. Students can modify structures and study the impact of modifications on the diffraction pattern. The analysis of simulated crystal illuminates geometric aspects of crystal structures.

Simulation of structures containing defects is a useful tool for the interpretation of diffuse scattering. Simulations allow fast and flexible realizations of complex defect models. The corresponding Fourier transform is readily calculated and can be compared to the observed data. New algorithms allow a quantitative analysis of diffuse scattering.

Participants will learn how to use the DISCUS program and create crystal structures and their corresponding Fourier- transforms for many applications that have proven highly efficient in our teaching experience.

The participants will be shown techniques related to crystal defects, analysis of diffraction patterns with Monte Carlo, and Reverse Monte Carlo methods. For more information, visit the website at http://www.uni-wuerzburg.de/mineralogie/crystal/workshop.html.

Highlighted Articles from IUCr Journals

John Helliwell, Editor-in-Chief of *Acta Cryst* and Chairman of the IUCr's Commission on Journals has arranged for reviews of articles in current issues of IUCr journals to appear in this and future issues of the IUCr Newsletter.

The Foundations of Macromolecular Structure Refinement

Techniques for macromolecular refinement continue to advance apace. The quality of data is improving with easier access to synchrotron sources, computing power is increasing while the cost is declining, and new algorithms are helping to put the calculations on a firmer statistical basis. In the past six months, three papers have appeared in *Acta Cryst.* A and D discussing the role of the normal matrix, the second-derivative matrix of the refinement target function.

The first problem to address is simply one of size; the normal matrix has the dimension of the number of parameters squared, and the time taken to generate it by classical techniques is proportional to the square of the number of atoms multiplied by the number of observations. The papers by Tronrud ["Efficient calculation of normal matrix in least-squares refinement of macromolecular structures", *Acta Cryst.* A55 (1999), 700-703]; Murshudov, Vagin, Lebedev, Wilson and Dodson ["Efficient anisotropic refinement of macromolecular structures using FFT", *Acta Cryst.* D55 (1999), 247-255]; and Templeton ["Faster calculation of the full matrix for least-squares refinement", *Acta Cryst.* A55 (1999), 695-699] all discuss ways of speeding up the calculations. These methods can be traced back first to Cruickshank who described an approach to refinement using Fourier methods in the 1950s [*Acta Cryst.* 5 (1952), 511-518; *Acta Cryst.* 9 (1956), 747-753], and then to Agarwal who showed how to exploit fast Fourier transforms (FFTs) [*Acta Cryst.* A34 (1978), 791-809]. He outlined a method for the fast calculation of second-derivative matrices, which is extended by Tronrud and generalized by Murshudov *et al*. Templeton extends another aspect of Agarwal's results, i.e., he makes approximations by replacing summations with integration assuming that the reciprocal space sampling is dense enough to justify this.

Most experience in exploiting the full normal matrix is in the field of small-molecule crystallography; here, it is feasible to generate the derivatives analytically, and to perform the inversion. When there is a high ratio of observations to parameters, its use has been shown to speed up the rate of convergence, and to reduce the likelihood of reaching a false minimum. When the refinement has converged, the inverse of the normal matrix reveals both the precision of the model parameters and the correlations between them. The eigenvectors and eigenvalues of the normal matrix provide information about parameters or parameter combinations that are not determined by the original data.

For large macromolecules, even if the full normal matrix is generated, there will be considerable problems in the inversion of such a large array. However, there are now many numerical tools developed within a variety of disciplines addressing such problems. The stability of the inversion procedure can be analysed using eigenvalues and -vectors, and this was discussed by Cowtan and Ten Eyck at the 18th European Crystallographic Meeting in Prague, Czech Republic in August 1998. They have performed such an eigensystem analysis on the normal matrices resulting from the least-squares refinement of a small metalloprotein using two datasets and models determined at different resolutions (all performed by classical techniques using the program SHELXL at the San Diego Supercomputer Center) [Sheldrick (1995), SHELXL93, a Program for the Refinement of Crystal Structures from Diffraction Data. Institut für Anorganische Chemie, Göttingen, Germany]. As a protein refinement is usually underdetermined without the application of geometric restraints, and these contributions are routinely included in the minimization residual, they have repeated their analysis including the contributions from such restraints. They show that the eigenvalue spectra reveal considerable information about the conditioning of the problem as the resolution varies. In the case of a restrained refinement, the spectra also provide information about the impact of various restraints on the refinement.

The established procedure used in macromolecular refinement programs such as SFALL/PROLSQ, XPLOR, and REFMAC has been to generate only the diagonal elements of the normal matrix for the X-ray data. Although this limits the rate of convergence, it does mean that each cycle is completed quickly because structure factors and gradients can both be generated using FFTs. All such programs incorporate the restraint derivative terms into the matrix, with some rather arbitrary weighting relative to the X-ray elements. The derivatives for these contributions can be generated simply, and provide off-diagonal terms for linked atoms only. Templeton's approximations for the maximum contribution for the X-ray off-diagonal terms show that these fall off rapidly with the distance between the atom pairs. Hence the geometric restraint contributions may well swamp any X-ray contribution to off-diagonal elements, especially when the resolution of the X-ray data is limited. But as Cowtan and Ten Eyck show, there are special situations where unexpected interactions link distant atoms, and these can degrade the course of refinement.

The FFT techniques for estimating the X-ray off-diagonal elements will make it possible to derive a much improved form for the full normal matrix in a realistic time, and we can look forward to further analyses, and a better understanding of the proper parameterization and accuracy of macromolecular structures.

Eleanor Dodson, U. of York, UK

Area Detectors - Current Trends and Why You Can't Have the Perfect Bucket

There are three factors that prevent you from owning the ideal area detector -the one with infinite count rate, zero dead time and unity detection efficiency out to 25 keV, namely:

* The "Laws of Physics" - don't ask for zero response time and zero noise floor.

* Available materials - it would be nice to have high-quality semiconductor wafers with absorbance coefficients of a few tens of micrometres for Eh = 3-30 keV and a direct bandgap so that only about a dozen electron-hole pairs are created per incident photon; but you've got silicon, gallium arsenide, indium phosphide and a few other esoteric materials with suspect mechanical properties.

* Current technology - the pressures on industry to develop faster 16-bit analogue-to-digital converters, faster and larger mass storage and a myriad of other components are driven by much bigger markets than protein crystallography (PX) instrumentation. We have to use what is available.

PX does not need an ideal detector for routine data collection. It has taken much discussion between practising crystallographers and detector experts to determine what is needed and what can be implemented.

It is a particularly interesting time to consider PX instrumentation, as the demand for quality data grows. The time chart for area detectors is film, wire chambers, image plates and, now, CCDs. Each new wave of detectors has to fight for acceptance by the community due to the slow transformation of a single prototype system into reliable, fully characterized, commercial products and, resistance to change. The current status of area detectors is illustrated by two recent papers in the *Journal of Synchrotron Radiation*. The first ["A multiple-CCD X-ray detector and its basic characterization", M. Suzuki *et al*., *J. Synchrotron Rad.*, 6 (1999), 6-18] describes a CCD mosaic system developed for the RIKEN beamline at SPring-8 (Hyogo, Japan). As scintillator-taper-CCD systems have become readily available, the drive has been to increase the aperture dimensions by stacking together single CCD systems to form close-butted mosaics. The RIKEN 4 x 4 CCDs provide a total aperture of 200 mm x 200 mm, giving resolutions out to approximately 2 Å at 12.4 keV. Smaller mosaics are becoming available commercially, but a 4 x 4 mosaic is large. As the paper rightly states, there are clear advantages in using more tapers with smaller demagnification ratios, as this will markedly improve sensitivity. The paper also highlights many of the practical issues necessary to achieve the very high levels of performance now possible with CCD systems. Suzuki *et al*.'s use of nonstandard CCDs, to reduce cooling requirements, will reduce the saturation charge capacity of the detector and the implications of this on the dynamic range for data collection remains to be seen.

Single CCD systems will continue to revolutionize small-crystal work and the capabilities of the home lab. Whether the trend of today's SR detector becoming tomorrow's home detector will persist depends on the fourth factor, which I forgot earlier: can you afford it? Multiple CCD systems and the pixel detectors are unlikely to fall to a price that the home lab could justify. The future for the home lab, in terms of reasonable cost and appropriate performance, may be with amorphous detectors.

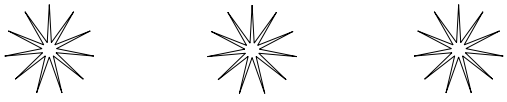
Just as CCD systems are becoming the workhorse for SR PX stations, the long-awaited solid-state pixel detectors are being subjected to immense development efforts by many groups at several SR sites. Their promise is both of photon counting and of continuous read-out.

The second paper ["X-ray powder diffraction with hybrid semiconductor pixel detectors", S. Manolopoulos *et al*., *J. Synchrotron Rad.*, 6 (1999), 112-115] reports the first application of a silicon pixel detector at an SR facility and the recording of preliminary powder diffraction data. The detecting device employed was small, not designed for SR use and had large dead times but it demonstrates the feasibility of such an approach, that interpixel dead spaces are probably not going to be as big a problem as some suggest, that good spatial resolution is attainable and that the detector survived!

My own views are, for SR facilities, that solid-state pixel detectors will become - after much expense, redesign and assessment - the preferred detector for many applications where crystal dimensions are relatively large (about 0.5 mm) as it will be difficult to reduce individual pixel sizes much below 150 μm. It is not their photon-counting capability, but their high-speed read-out, which will open up opportunities for new dynamic experiments and close the gap between potential sample fluxes and detector count-rate limits.

For the foreseeable future, pixel detectors will not possess unity quantum efficiency across the whole energy range. It is worth rehearsing the arguments for integrating vs. photon-counting detectors - for CCD vs. pixel detector. We can consider the individual CCD pixels as buckets that are filled, over the frame time, by photon-generated electrons. So integrating detectors are where you let the balls (electrons) fall into a bucket for a given time, and just before you empty the bucket so you can count the balls (to calculate the balls caught per second), some demon - who represents the read-out and system noise - throws a random number of balls into the bucket. Ideal photon-counting detectors allow you to count balls individually as they fall into the bucket. For practical solid-state pixel detectors, the problem is a fraction (and you are never certain exactly what the fraction is) of the balls miss the bucket completely - this is particularly so for high-energy balls, which pass straight through the bucket, - or, even more amazingly, a ball may split in two with each half landing in different buckets. These do not get counted at all and this is bad news for low-energy balls. So we will not get the ideal bucket (i.e., detector) but we will with pixel detectors get a better bucket - one that matches closer our specification envelope. Thus the second paper is brief but a flag-planting one as it demonstrates the way forward to a whole new range of buckets and a whole new range of science.

Nigel M. Allinson, UMIST, Manchester, UK



Four-Circle Diffractometer for Sale

Siemens/Nicolet P3 four-circle X-ray diffractometer for sale. 3 kW solid-state generator driving a sealed X-ray tube, a MicroVAX host computer and an extended two-theta arm. 9 years old, maintained under contract throughout, in excellent condition. Suitable for a small-molecule crystallography lab.

Will consider any reasonable offer. Contact: S.E.V. Phillips, School of Biochemistry and Molecular Biology, U. of Leeds, Leeds LS2 9JT UK, e-mail: S.E.V.Phillips@Leeds.ac.uk

New CIF Dictionaries

The last report from the committee appointed by the IUCr to oversee the CIF project, Comcifs, described the current status of the core (coreCIF), powder diffraction (pdCIF) and macromolecular (mmCIF) dictionaries, and gave details of the three dictionary maintenance groups that have been established to continue their development (IUC Newsletter Vol.6 No.4 page 6).

New specialized CIF dictionaries to cover branches of crystallography not covered are being prepared. Once provisional approval has been given, the draft dictionaries will be made available on the web for public input. Final approval of the dictionary usually occurs after potential users have had a chance to comment and suggest changes. Below is a summary of the current state of the dictionaries under development. Anyone interested in contributing to them should contact the project leader.

MODULATED STRUCTURES (msCIF.dictionary) Project leader: G. Madariaga (wmpmameg@lg.ehu.es) This dictionary will provide the data items needed to give a complete description of modulated structures. It is in an advanced state of preparation and will shortly be presented to Comcifs for provisional approval.

IMAGES AND HIGHER DIMENSIONAL DATA (imgCIF/CBF) Project leader: A. Hammersley (hammersley@esrf.fr) The purpose of this dictionary is image storage. Initially the focus is on 2-D image data-sets, but the dictionary will be flexible enough to allow storage of multi-dimensional data-sets. To encode the large amount of information needed to define an image in a way that made reading and writing the file efficient, the group decided that the image had to be written in binary. Unfortunately, this contravenes the basic premise that all cifs are written in ASCII. Consequently, a CBF (Crystallographic Binary File) will be used for file transfers between computers, while the fully cif compliant imgCIF written in ASCII will be used for archiving. Both files use identical data names and definitions and have the same structure. The only difference is that CBFs are written as binary files and imgCIFs are written as ASCII files. H. Bernstein and P. Ellis have been working on software that will convert one into the other. This dictionary will be coming to Comcifs for tentative approval within the next few months.

SYMMETRY (symCIF.dictionary) Project leader: D. Brown (idbrown@mcmaster.ca) The purpose of this dictionary is to define all the symmetry items that are needed to describe the contents of International Tables Vol A and to provide a framework in which, for example, tables of sub- and super-groups can be expressed.

DIFFUSE SCATTERING (dsCIF.dictionary) Project leader: T. Proffen (proffen@pa.msu.edu) Currently identifying the concepts needed in a diffuse scattering dictionary.

ELECTRON DENSITY (rhoCIF.dictionary) Project leader: P. Mallinson (paul@chem.gla.ac.uk) This dictionary will provide the data items needed for reporting the results of electron density studies.

SMALL ANGLE SCATTERING (sasCIF.dictionary) Project leader: M. Malfois (malfois@embl-hamburg.de) A draft dictionary describing the items needed in the small angle scattering field.

MAGNETIC STRUCTURES (magCIF.dictionary) Project leader: W. Sikora (sikora@novell.ftj.agh.edu.pl) This dictionary is being developed in conjunction with the establishment of an electronic version of the Database of Magnetic Structures Determined by Neutron Diffraction in Krakow.

The CIF dictionaries are copyrighted by the IUCr in order to protect the CIF standard. Any file that calls itself a CIF must comply with the standard laid down in these dictionaries. Anyone interested in expanding CIF into areas not covered, should contact the chair of Comcifs, D. Brown (idbrown@mcmaster.ca) or the secretary (B. McMahon, bm@iucr.org).

I.D.Brown Chair, Comcifs

ICSD Symposium at Glasgow

A symposium is being planned on 'Innovative Uses of the Inorganic Crystal Structure Database'. Topics will include:

•Structure and content: What information should the database contain? •Software and hardware: What are the best ways of delivering the information in the database? •New applications: eg. comparative structural chemistry, structure design and modeling, how will people be using the database in 20 years time?

X-Ray Research

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X-Ray Research

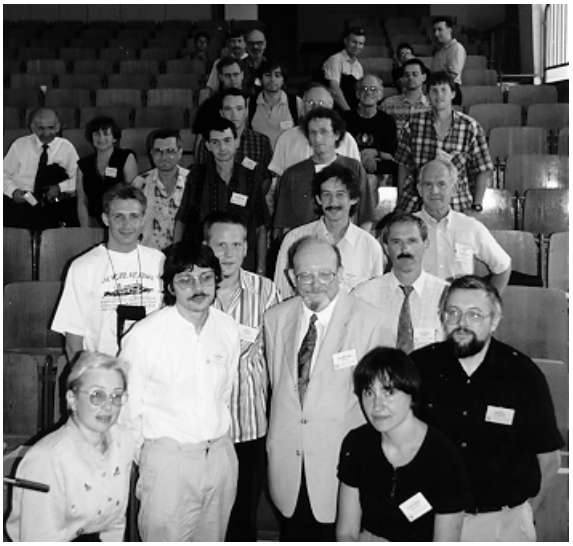
More from ECM 18, Prague

The microsymposium on INDUSTRIAL APPLICATIONS AT NEUTRON AND SYNCHROTRON SOURCES (A6) began with an overview on applications of neutron diffraction to materials science, ranging from residual stress to texture analysis and phase analysis in thick components (M. Daymond, ISIS). Other presentations concerned neutron diffraction at the Czech facility (P. Lukas,NPI), kinetics studies of the hydration process, online and X-ray diffraction to clinker quality control in cement manufactures (M. Bellotto, CTG) and energy-dispersive X-ray diffraction studies at Daresbury (P. Barnes, Birbeck College). P. Scardi described the new synchrotron radiation XRD station at Elettra (Italy) for thin film and surfaces anaysis of polycrystalline materials. [P. Scardi]

At the microsyposium on THE INTERNET IN CRYSTALLOGRAPHY (F2) G.J. Kearley and D. Richard (France) showed how the WWW can be used to provide a graphic user interface for running data analysis programmes on a remote central server (http://barns.ill.fr). The WWW server uses Java and the BARNS interface was demonstrated by video projection from a local computer running the server and the WWW client. G. Chapuis and W. Hardaker (France) demonstrated an interactive WWW course on crystallography "Discovering Symmetry" (http://www-sphys.unil.ch/symmetry/). H. Flack described the IUCr on-line information service (http://www.iucr.org/) L. Cranswick (UK) demonstrated his NEXUS CD-rom collection of the best of the crystallographic internet (http://www.unige.ch/crystal/stxnews/nexus/index.htm). F. Allen (UK, http://www.ccdc.cam.ac.uk/) said that the CSD can be accessed *via* the Internet under controlled circumstances within certain countries. A. Hewat (ILL) described the ICSD-for-WWW interface (http://www.ill.fr/icsd) which allows full access to the Inorganic Crystal Structure Database *via* a graphic user interface and the tools for generating 3D drawings, indexed plots of powder patterns, bond length and valence-bond calculations. [*A. Hewat*]

In a discussion session on STRUCTURAL BIOLOGY IN CENTRAL AND EASTERN EUROPE (F4), E.N.Baker described establishing macro-molecular crystallography in New Zealand in the 1970s. His list of required resources included a supportive biological community, collaborators, politicians, and funding agencies; an accessible problem; helpful, innovative and enthusiastic students; essential in-house equipment (X-ray generator, crystal freezing, computing); access to synchrotrons and travel money. Structural biology initatives in Europe were described by M. Jaskolski (Poland), J. Sevcik (the Slovak Republic), D. Turk (Slovenia), B. Schneider (Czech Republic), B. Kamenar (Croatia) and V. Harmat (Hungary). In Poland, Slovenia, Hungary and the Czech Republic, the equivalent of 400,000 - 500,000 $US was used to set up structural biology groups. Sustained efforts will require economic stability, sustained interest of the biological community, salaries sufficient to attract and keep young people, an industrial sector willing, and able, to collaborate in and finance research; a fund to maintain the equipment, and attract scientists from abroad. There is a need for collaboration within the east European countries and continuing support by western Europe. Possible source of financial support for Structural Biology in Central and East Europe discussed included the EC, INTAS and COPERNICUS programs; the UK Royal Society, NATO, the Soras Foundation, Howard Hughes, ESF and EMBO. The participants of the Microsymposium agreed to form a consortium of macromolecular crystallography groups across Central and Eastern Europe. (M. Jaskolski, Poland, chair) to reinforce collaborations between these countries and to promote their interests within Europe. [*A. Lewit-Bentley*]

P.G. Radaelli at the ECM microsymposium on Magnetic Materials. He will give a plenary lecture in Glasgow (Photo WLD)



Speakers (A. Pobokov, V. Klemm, M. Drakopoulos, R. Barabash, H. Leipner, M. Chall, and O. Zahararko) join their audience at the Defects and Microstructure microsymposium at ECM18. (photo WLD)

D. Schwarzenbach began the session on TEACHING CRYSTALLOGRAPHY (F8) with a discussion of how to teach crystallography to different students (physicists, chemists, mineralogists and materials scientists) and raised the question "What is basic crystallography?" which led to a lively discussion of symmetry and Bragg´s law. Other symposium topics included: "An Interactive Book on Crystallography" (G. Polidori), "Crystallography for Geologists: Twenty Years Later" (D. Yu. Pushcharovsky) and "Teaching Crystal Growth as an Educational Activity in Crystallography"(N. Leonyuk). C.M. Gramaccioli discussed the significance of symmetry in spectroscopy and quantum mechanics and the central role that crystallography plays in solid state physics and chemistry. K. Crennel, discussed "Educational and Teaching Activities of the British Crystallographic Association", which are reflected in the BCA home pages: URL http://gordon.cryst.bbk.ac.uk/BCA/index.html. [*A. Oskarsson*]

Martensitic Phase Transformations The Memory of Shape

The Middle Age Knights used to heat their swords in fire and quench them in cold water; after that, the swords became much harder. This method has long been used in the steel industry. The hardening comes from a characteristic microstructure formed by quenching, which is denoted by the term *martensite* in honour of the German metallographer A. Martens. Initially, the term was ambiguously adopted to denote the microstructure of quenched steels, but, as the nature of this microstructure became better known, the meaning of the word has been gradually clarified and extended to other alloys. The process (a phase transformation) by which the martensite is obtained is a *martensitic transformation* (MT). This is a first order solid-solid phase transition with displacive nature (without atomic diffusion) consisting of a homogeneous lattice deformation leading to the new crystal structure. The interface between the parent phase (austenite) and the product phase (martensite) is constituted by an invariant plane denoted as the habit plane (in general, with irrational Miller indices). The transformation proceeds by the movement of the habit plane. Due to the displacive character, the transformation proceeds by small cooperative movements of the atoms, keeping the same chemical composition and atomic order of the parent phase. In addition to a change in the crystal symmetry, the transformation brings about a deformation (mainly a shear on the habit plane) as well as a volume change. From a crystallographic point of view, the change of crystal structure takes place by a homogeneous lattice deformation, but an additional lattice invariant shear, occurring by slip or by twinning, together with a rigid-body rotation also have to be considered in order to keep invariant the habit plane. From a given orientation of the parent phase, several variants of martensite with different orientations are possible.

The MT can be induced by changing the temperature (on cooling) or by applying an external stress. The transformation temperatures (or stresses), which can cover a wide range from ~ 0 K to - 600 K are mainly dependent on alloy composition, but other factors (atomic order, internal stresses, lattice defects) also influence them. In general, the transformation is reversible, the reverse transformation takes place by heating from the martensitic state or by releasing the stress, but it proceeds at higher temperatures or lower stresses than the direct transformation, thus the transformation cycle exhibits hysteresis. The temperature induced transformation develops a multivariant martensitic microstructure with self-accommodation, *i.e.* the deformation associated with one martensite plate is compensated by the neighbour variant, not giving a net macroscopic shape change. On the contrary, a limited number of variants form by the stress induced transformation, those variants which deform the material in the sense of the applied stress. Two types of martensitic transformations can be distinguished. The *burst-type* transformations, typical of the quenched steels, occur almost isothermally and are characterized by a big volume change and a wide hysteresis (hundreds of K). The *thermoelastic martensitic transformations* have a small volume change, low hysteresis (tens of K), and good reversibility. The deformation accompanying the transformation is almost completely elastically accommodated but, due to this elastic energy, a continuous cooling is needed in order to complete the transformation.

Thermoelastic martensitic transformation's (TMTs) occur in Au-Cd, In-Tl, Ni-Ti, some Cu-based alloys and other systems. Due to

Speakers at the microsymposia "Martensitic Transformations" include T. Goryczka, H. Morawiec, V. Novak, P. Sittner, T.V. Novoselova, N. Gu, J. Pons, E.N. Dzevin, A.I. Taluts and L.O. Andruschik. (Photo WLD)

TMTs and especially reverse transformation, alloys exhibit un-usual thermomechanical behaviours and shape memory capabilities. For that reason they are referred to as *shape memory alloys* (SMA). If a SMA initially in the parent phase condition is cooled to the martensite phase, nothing occurs macroscopically, but if an external load is applied, the piece is deformed in an apparent plastic way (the deformed shape remains after the load is released). In fact, the deformation takes place not by the movement of dislocations, but by a reorientation of the martensite variants towards those favored by the external load. If the piece is heated up till the reverse transformation takes place, the parent phase crystal structure and shape is spontaneously restored. It seems that the material "remembers" its original shape and spontaneously adopts it when heated through the reverse transformation. This is the *shape memory effect*. If the piece of SMA is loaded in the parent phase condition the martensitic transformation is stress induced, which brings about a large deformation (up to 10% elongation in well oriented single crystals). If the applied stress is not so high as to produce plastic deformation of the martensite, the induced deformation is completely recovered by the reverse transformation when releasing the external load. So, the material can be largely deformed in an apparently elastic way. This property is called *pseudoelasticiy*. The *two-way shape memory effect*, in which the material changes spontaneously its shape also on cooling, can also be induced after a suitable training treatment. Many applications of the shape memory properties have been developed, especially for Ni-Ti, and the Cu-based alloys. SMA's can be used as temperature sensors, but do not offer great advantage over standard ones. SMA's have advantage as actuators (the movement and force available are used to do some action) and as connectors for pipes and wires with vibration protection. They have applications in robotics (movement of arms and fingers), medicine (orthodontics, guide wires for catheters, surgery implants) and the car, aerospace and nuclear industry.

In the ECM-18, microsymposium a wide range of topics in this field were presented, starting with a review of the phenomenological crystallographic theories for MT, pointing out their limitations. From a crystallographic point of view, the theories describing the MT are phenomenological and little knowledge exists on the exact movement of the atoms to develop the new phase. In this subject, the Crystallography community can make a fruitful contribution.

Jaume Pons

Indian World of Crystallography

The 270 papers presented at the XXIX National Seminar on Crystallography at the Dept of Crystallography and Biophysics, U. of Madras, Guindy Campus in Dec. 1998 covered crystallographic applications to biomedicine and material science, biocrystallography, organic, and inorganic structures, physical properties, crystal growth and characterization. K. Lal, treasurer of the Asian Crystallographic Association opened the meeting. A highlight of the meeting was a talk C.N.R. Rao, F.R.S. on "Crystallography in the Study of the Chemistry of Materials". Other highlights included sessions on Synchrotron Radiation, weak interactions, polymeric network design, supramolecular organic metal coordination complexes, smart materials, graphite nanotube formation, characterization of nanoparticles, high temperature and high pressure studies.

V. Pattabhi

XXIX National Seminar on Crystallography. (Photo courtesy of V. Pattabhi)

Chemical Crystallography in Latvia

A meeting honoring Latvian crystallographer and chemist M.E. Straumanis was held at Riga Technical U. on the 100th anniversary of Straumanis's birth (Nov. 23, 1898) with support from the Latvian Academy of Sciences, Latvian Chemical Society and Latvian Crystallographic Assoc. Straumanis received an engineer-chemist degree from Latvian U. in 1925, a PhD degree in 1927 and a Rockfeller fellowship. From 1931-1935 Straumanis and A. Ievins developed a method for accurate lattice parameter measurement known as the "asymmetric Debye-Scherrer method". From 1944-1947 he studied metal corrosion at Marghburg U. (Germany) before taking up a positon at school of Mine and Metallurgy, Missouri U. (USA) where he continued studies on titanium, zirconium, halfnium and thorium interactions with acids. In 1967 the electrochemistry lab at MU was named the Straumanis Lab for Electrochemical Studies. He published more than 300 papers and was a co-authors of "50 years of X-ray Diffraction." The meeting included lectures on Straumanis' contribution to crystallography and other fields and reports of X-ray studies carried out by Latvian crystallographers in the field of inorganic and organic chemistry. A special issue of the *Latvian Chemical Journal* N3, 1998 has been devoted to Straumanis 100th anniversary.

A. Mishnev, Latvian Crystallographic Assoc.

A space group of participants at the 7th Conference of SCS in September, 1998. Photo courtesy of D. Poleti)

Serbian Crystallographers

After the disordering of the previous Yugoslavia, crystallographers in Serbia recrystallized as the Serbian Crystallographic Society (SCS) in the spring of 1992. The cell of the SCS contains 80 members from Serbia and Montenegro working in crystallography and related fields through different symmetry operations. The asymmetric unit contains a 25 scientists hard-core acting as seeds for all investigations. The SCS belongs to the IUCr through the European Crystallographic Association subgroup. Since 1992 the September Conference of SCS has grown to three days and includes formal sessions (opening ceremony and plenary lecture), three working sessions, a half-day excursion and, the conference dinner. A book of one-page abstracts (CIF format not accepted!) has been printed every year. Plenary lecturers from abroad, A. Kalman, G. Argay (Budapest, Hungary), A. Spasoevic-de Bire (Paris, France), N. Furmanova (Moscow, Russia) and R. Tellgren (Uppsala, Sweden) presented well-ordered lectures. We hope that they enjoyed our lattice. The seventh-fold conference was held in Vrnjacka Banja a well-known spa in Sept. 1998. A limited number of conference reports are available free of charge (in English and Serbian), contact L. Karanovic (ljika@helix.chem.bg.ac.yu). The Eighth-fold conference will be held in the first half of Sept. 1999 in Kragujevac.

D. Poleti

J Schneider

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Participants at the ACA Summer Course. (Photo courtesy of ACA)

ACA Summer School

The seventh annual ACA Summer Course in Crystallography, U. of Georgia, July, 1998 offered instruction and hands-on training in small molecule X-ray diffraction and fundamental training in macromolecular crystallography. 60 graduate and undergraduate students, post-docs and representatives from industrial laboratories attended. IUCr Travel Scholarships were awarded to C. Arici (Turkey), E. Baez (Mexico), D. Lecerof (Sweden), S. Ozcan (Turkey), A. Teplitsky (Israel), and W. Tempel (UK). The course was dedicated to the memory of K.N. Trueblood one of its founders. The course offered lectures on fundamentals during the mornings, hands-on Lab experience during the afternoons and lecturers on more advanced topics in the evenings. The staff included W. Cordes, B. Craven, S. Geib, H. Hauptman, R. Marsh, G. Newton, W. Robinson, J. Rose, R. Sparks, C. Campana, D. Frankel, K. Tesh, and D. Stewart. The last four days focused on macromolecular crystallography including crystallizations, data collection strategies, derivative preparation, isomorphous replacement, anomalous scattering and various structure refinement methods. Lecturers included L. DeLucas, W. Furey, L. Lipscomb, Z. Liu, C. Momany, B.-C. Wang, C. Chen, S. Foundling, A. Wang, and C. Wu. Students received the fourth edition of the lecture outline "Structure Analysis by X-ray Crystallography". Sponsors included the U. of Georgia, the ACA, the IUCr, Molecular Structure Corp, Nonius, Bruker and MarResearch provided lecturers, lab tutors, consultants and two scholarships each. Next years school, July 13-28 will include eight days of fundamental and small molecule crystallography and eight days of macromolecular crystallography.

G. Newton

Microgravity Gets Off the Ground in Granada

Nearly 250 scientists from academia, government, and industry gathered for the Seventh Int'l Conference on the Crystallization of Biological Macromolecules, in May 1998 in Granada, Spain. A highlight of the session on microgravity was a plenary talk titled "Recent Advances in Microgravity Crystallization of Biological Macromolecules," given by Principal Investigator, A. McPherson, of the U. of California, Irvine. During the microgravity session, Lawrence DeLucas, of the U. of Alabama, Birmingham, also presented papers titled "X-ray Facility for the Int'l Space Station" and "Vapor Diffusion Crystal Growth Experiments in Microgravity."

(from Microgravity News Summer '98)

Electron School

The 4th Stockholm Electron Crystallography School took place during Midsummer week 1998. Students came from 20 countries on all 5 continents. The external teachers were J. Steeds, Bristol (CBED), B. Cernik, Daresbury Synchrotron (Powder Diffraction), L. Marks, Chicago (surface structures) and G. Cascarano (direct methods for solving structures from SAED data).

(Electron Crystallography News August '98)

ICDD 2000 Scholarship Awards

The science of crystallography has played a key role in the development of X-ray diffraction, electron diffraction and neutron diffraction for the elucidation of the atomic structure of matter. Crystallography is an interdisciplinary branch of science taught in departments of physics, chemistry, geology, molecular biology, metallurgy and material science. To encourage promising graduate students to pursue crystallographically oriented research, the International Centre for Diffraction Data (ICDD) has established a Crystallography Scholarship Fund. While the Ewald Prize is awarded every three years to an internationally recognized crystallographer, little effort has been made by science departments to cultivate aspiring crystallographers. Convinced of the beneficial, scientific impact of the proposed scholarships for crystallographically oriented research, the ICDD has solicited funds from private and industrial sectors to support this program. The ICDD has awarded twenty-eight scholarships in the amount of $2,000 each since 1992. The year 2000 Scholarship Award has been increased to $2,250.

Qualifications for the applicant: The applicant should be a graduate student seeking a degree with major interest in crystallography e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. There are no restrictions on country, race, age or sex. The term of the scholarship is one year. The recipient may make application for one renewal at the end of the first year. Because a limited number of scholarships are awarded, renewal applications will be considered on a competitive basis in conjunction with all applications that have been submitted up to the closing date.

Submit: •Curriculum Vitae, listing degree(s) held and degree(s) sought. •A one page proposal by the graduate student describing the type of crystallographic research to be partially supported by scholarship. •A supportive letter from the sponsoring professor of an accredited university or an institute of technology on institution letterhead.

Restrictions on the scholarship fund: •The scholarship stipend is to be used by the graduate student to help defray tuition and laboratory fees. A portion of the stipend may be applied to registration fees to accredited scientific meetings related to crystallography. •No more than one scholarship will be awarded to applicants at any one accredited institution per year. •The funds of the scholarship are not to be used for travel. A committee consisting of the ICDD Chairman, the Chairman of the ICDD Technical Committee, the Chairman of the ICDD Education Subcommittee, and three or four individuals without conflict of interest administer the awarding of the scholarships. One or more accredited professors (with no conflicts of interest) may be invited to assist in the selection of successful candidates.

Applications must be received by Oct. 29, 1999. Please mail to:Secretary, ICDD, 12 Campus Boulevard Newtown Square, PA 19073-3273 USA.

The PDB has a New Home

On Oct. 1, 1998 the Research Collaboratory for Structural Bioinformatics (RCSB), a consortium composed of Rutgers, the State U. of New Jersey; U. of California San Diego/San Diego Supercomputer Center (SDSC); and the National Inst. of Standards and Technology (NIST), received a five-year award to manage the Protein Data Bank (PDB). The project will run under a Cooperative Agreement from the National Science Foundation (NSF), with funding from that agency as well as the Dept. of Energy, and two units of the National Institutes of Health: the National Inst. of General Medical Sciences and the National Library of Medicine.

The RCSB has created a system with higher, faster throughput of deposited data; a greater number of query capabilities, including more complex and specific queries; a uniform archive; dynamic cross-links to other databases; and the availability of structure and sequence neighboring. The PDB data will be stored and mirrored at all three RCSB sites and at key sites worldwide.

Principal investigator H. Berman heads the RCSB team at Rutgers which includes J. Westbrook, who has played a key role in the development of the mmCIF dictionary. At the San Diego Supercomputer Center (SDSC) at UCSD, P. Bourne leads a group of scientists in a Biological Data Representation and Query initiative. Together with P. Arzberger, a computational biologist and Executive Director of NPACI, this group will be responsible for all aspects of data query and distribution. G.L. Gilliland, chief of the Biotechnology Div. in NIST's Chemical Science and Technology Lab, will lead the NIST effort to establish data uniformity, improve the accessibility and reliability of queries, and manage the Master Archive.

The RCSB is working with the Brookhaven National Laboratories (BNL) team headed by J. Sussman to ensure that there is a seamless transition that will be completed by Oct. 31, 1999. A website (http://www.rcsb.org) has been established to provide up to date transition information and to provide access to the new features of the system as they become available.

Helen Berman, Gary Gilliland, Phil Bourne
From ACA Newsletter

International Collaboration

Grants are available to individual American specialists who plan to establish new research partnerships with their colleagues from Central/Eastern Europe (CEE) and the Newly Independent States (NIS). This program is designed primarily to prepare these new partnerships for competition in NSF programs. Two types of grants are available. Short-term: to support American specialists who wish to host or visit their CEE or NIS colleagues for two-week periods in order to prepare collaborative research proposals for submission to NSF. Long-term: visits last from one to six months and significant joint publications are expected. Postmarking deadlines for proposals are April 5, 1999 (project development only), July 30, 1999 (long-term only) and Aug. 16, 1999 (project development only). For more information contact http://www2.nas.edu/oia/22da.html

Teaching Tools: Lab Manual for Shelxtl

A step by step guide to solving routine crystal structures for crystallographic novices and is entitled "Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction" is available free of charge as a .pdf file to academic users who will only be required to register their copies and keep me informed of how it is used in their teaching. If you are interested in obtaining a copy, please contact me at adhunter@cc.ysu.edu.

Allen Hunter

ICSD

ICSD is now cooperatively produced by FIX Karlsruhe, the Max-Planck Society (MPG) and the US Nat'l Inst. For Science and Tech. (NIST). At present, the distribution of the tasks between the three partners is as follows: •production, distribution and marketing by FIZ Karlsruhe, •quality control by MPG, •development of new inhouse and other software as well as evaluation by NIST.

On the Cover:

Clockwise beginning at upper left:

1) Ribbon drawing of FepA, an active transporter of ferric enterobactin in the outer membrane of *E. coli*. S.K. Buchanan *et al*. (1999*) Nature Structural Biology* 6:56. *Courtesy of Hans Deisenhofer*, 2) Neutron quasi-Laue diffraction pattern from tetragonal hen egg-white lysozyme revealed 960 hydrogen atoms and 251 water molecules. N. Niimura, *et al.*, *Nature Structural Biology*, Vol.4, No11, 1997, pp909-914. *Courtesy of N. Niimura*; 3) Anisotropic Displacement Parameters (ADP) of anthraquinone between 160 and 300K (Brock and Fu, *Acta Cryst.* B54 (1998) 308) shows butterfly-type motion of the molecule (S.C. Capelli, Ph.D. thesis, U. of Bern, Switzerland, 1999). Picture by J. Hauser. *Courtesy of H.-B Bürgi*; 4) A 24-nucleotide RNA enzyme, Leadzyme, complexed with $Sr(H_2O)_3$(II) at 1.8 Å resolution reveals how small ribozymes recruit metals to activate specific 2'-hydroxyl groups for nucleophilic attack leading to phosphodiester scission. The substrate has a purple electron density surface and yellow nucleotide bonds. The ribozyme, a yellow electron density surface and pink nucleotide bonds. *Courtesy of David McKay*; 5) The hydrate of 18-crown-6/methylammonium fluoride, a channel structure in which water molecules form a 'double helix' along the crystallographic z axis. *Courtesy of Janusz Lipkowski*; 6) A model of a surfactant templated silicate structure at the air water interface of a cetyl trimethyl ammonium solution being studied by X-ray and neutron reflectivity. *Courtesy of John White*; 7) A very-large-pore high-silica zeolite UTD-1 bis(pentamethylcyclopentadienyl)cobalt(III) complex solved *ab initio* from powder diffraction data collected on a textured sample. *Courtesy of Lynne B. McCusker*; 8) The end of the myosin power stroke from crystal structure analysis of actin and myosin and electron microscopy of the actin-myosin complex. *Courtesy of Ken Holmes*.

Frank G. Foote (1906-1998)

Frank G. Foote, Principal Metallurgist at the Manhattan Project's Metallurgical Laboratory and former Director of Argonne Nat'l Laboratory's Metallurgy Division, died on Nov. 17, 1998. Foote received a master's degree in chemistry from Ohio State in 1930 and a doctorate in metallurgy from Columbia U. in 1941. His principal research interest was the study of the structure of solids by x-ray diffraction; his and E.R. Jette's paper on the defect structure of FeO, published in volume I of the *Journal of Chemical Physics*, is a classic. Foote joined the Manhattan Project in Chicago in 1943. In May of 1946, Foote returned to the School of Mines of Columbia U. He returned to Argonne as director of the Metallurgy Division (1948-1966). He believed that the study of highly anisotropic materials such as uranium and plutonium would yield insights not obtained from studies on materials of higher symmetry, and enthusiastically supported basic research on U and Pu, production of pure materials, growth of single crystals, measurements of elastic, electrical, magnetic and structural properties, deformation mechanisms, alloy phase diagrams, radiation damage, corrosion, etc. He presented a review of this work at the 1955 Atoms for Peace Conference in Geneva. Frank Foote was a fellow of the AAAS and the American Nuclear Society, and a member of the American Society for Metals, the American Institute of Mining, Metallurgical, and Petroleum engineers, the American Physical Society, and the ACA. He was a quiet scholarly, kind man. He never lost his interest in science or the people he worked with. He is remembered for his sterling qualities, and for his leadership in one of the most exciting periods of science and technology in American history.

Evgeny Konstantinovich Vasil'ev (1922-1999)

Evgeny Konstantinovich Vasil'ev, prominent scientist, X-ray physicist, senior colleague of the Inst. of the Earth Crust of the Siberian Branch of the Russian Academy of Sciences (IEC SB RAS), a member of the Siberian Branch of the RAS, and a Doctor of Philosophy died on March 5, 1999 at the age 76.

He was born on September 8, 1922 in the village Zhigalovo, Irkutsk, Russia and began his study at the physical and mathematical faculty of Irkutsk State U. (ISU) in 1940. His education was interrupted by the Second World War, when he served in the Red Army. After the war he graduated from the ISU with honors in 1949 and he worked at the Irkutsk Inst. of rare metals (1949-1950), the East Siberian Geological Inst. of the RAS, which was renamed the Inst. of the Earth Crust in 1962. From 1955 until his death, Vasil'ev worked in the IEC SB RAS. In 1965 he completed his Ph.D. thesis: "Application of the mathematical statistics methods to X-ray diffraction study of an isomorphic series of olivines and garnets".

Studying minerals at the diamond provinces in Yakutia, his highly productive group discovered and characterized new minerals, including florensovite, olekminskite, azoproite, tazheranite, zemkorite, and odintsovite. Rapid X-ray diffraction methods for mineral identification were developed under his direction were the first conducted in East Siberia. He also developed protocols for X-ray powder diffraction data analysis in Russia. Vasil'ev is an author and a co-author more then 150 scientific works including 6 monographs and his book "Qualitative X-ray phase analyze".

He was on the faculty of the Irkutsk State U., a member of the Commission of X-ray diffraction analysis, the Russian Mineralogical Society, the working group on crystal structure and mineralogical databases of KODATA, the editorial board of the "Powder Diffraction", organizing committees of many national and international conferences. and significant contributor to the ICDD.

Vasil'ev was well organized, highly productive, diligent, inquisitive, generous and caring. He will be remembered as a scientist, a remarkable person and our colleague.

Vladimir Evsyunin, Anatoly Revenko, Anvar Kashaev

Emil Harutyunyan (1935-1998)

Prof. Emil Harutyunyan, Russian protein crystallographer, died in Moscow on Oct. 8, 1998, at the age of 62.

Emil was born on Oct. 10, 1935, in Erevan. He graduated from the Erevan State University in 1957 and joined the Instituted of General and Inorganic Chemistry of the Russian Academy of Sciences in Moscow as a post-graduate student, where he was supervised by Mikhail Porai-Koshits. His Ph.D. Thesis was devoted to X-ray diffraction study of a series of uranium and thorium compounds.

In 1966, Emil began his work in the Institute of Crystallography at the Lab. of Biocrystal Structures with Boris Vainshtein. He was one of the pioneers in X-ray protein crystallography in Russia. Emil took an active part in solving the first three-dimensional protein structure in Russia, namely, the structure of the oxygen-binding plant protein leghaemoglobin, at high resolution. The three-dimensional structures of inorganic pyrophosphatase, formate dehydrogenase, and a number of pyridoxal-dependent enzymes, were determined under his supervision. His research in X-ray crystallography resulted in the publication of about 150 journal articles.

He was a very good teacher. Fourteen young scientists supervised by Emil, received their Ph.D., and are presently working in the best protein crystallography laboratories of the world. After the death of Boris Vainshtein in 1996, Emil succeeded as Head of the Lab. of Biocrystal Structures at the Institute of Crystallography. In spite of the troublesome times, he acquired research facilities, tirelessly fostered a collaborative atmosphere in the laboratory, and contributed substantially to the development of protein crystallography in Russia.

Emil was a scientist of unique research talent and an amicable person. He was always cheerful and enthusiastic. He was not afraid to take up the most ambitious problems and never failed to implement them with success. He will remain in our grateful memory forever.

William Melik-Adamyam and Tatiana Safonova

Oxford Cryosystems

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Pittsburgh Diffraction Conference

The 57th Annual Pittsburgh Diffraction Conference will be held at Ohio State U., Columbus, Ohio Oct. 21-23, 1999. This year the main symposium, entitled "From Nucleic Acids to Proteins", will be in honor of Prof. M. Sundaralingam in celebration of his four decades as an X-ray crystallographer. The symposium is being organized by M. Caffrey (caffrey@chemistry.ohio-state.edu) and R. Rubin (rubinj@aa.wl.com). There will be an additional symposium entitled "Crystal Growth" which is being organized by G. DeTitta (detitta@hwi.buffalo.edu).

For continuing conference updates, see http://www.pitt.edu/~geib/pds.html. General inquiries should be addressed to the Conference Chair, B. Craven (craven@grove.iup.edu).

Physical Methods in Coordination and Supramolecular Chemistry

The XIII International Conference "Physical Methods in Coordination and Supramolecular Chemistry" will be held Sept. 7-10, 1999 in Chisinau, R. Moldova. N. Gerbeleu (R. Moldova) is chairman and J. Lipkowski, (Poland) as co-chairman.

Invited speakers include: S. Andronati (Ukraine), M. Antipin (Russia), J.-L. Atwood (USA), A. Garnovskii (Russia), G. Gokel (USA), I. Goldberg (Israel), I. Haiduc (Romania), M. Fonari (R. Moldova), G. Kamalov (Ukraine), Yu. Kokunov (Russia), V. Kravtsov (R. Moldova), V. Leovac (Yugoslavia), J. Lipkowski (Poland), L. Mazalov (Russia), V. Nefiodov (Russia), Yu. Simonov (R. Moldova), Gr. Timco (R. Moldova), C. Turta (R. Moldova), and M. Zaworotko (Canada).

Topics addressed with include magnetochemistry and resonance methods (NMR, ESR, NCPR, Mossbauer spectroscopy etc.), fundamental problems of Coordination and Supramolecular Chemistry, application of spectroscopy (X-ray radiation, circular magnetical and optical dichroism, Raman scattering, of atomic circular polarised emission) to the study of Coordination and Supramolecular Compounds. The Investigation of the structure and reactivity of Metalocomplexes in the gas phase, using Mass Spectrometry, Photoelectron XPS and UPS spectroscopy, IR and UV vacuum spectroscopy etc., Original techniques in Coordination and Supramolecular Chemistry.

The deadline for applications is June 1, 1999 The official language of the Conference is English. Registration is $100 (participants from Eastern Europe countries and the former USSR -$20), students are $50 ($10 for East Europe countries and ex-USSR). Entrance visa for Republic of Moldova can be obtained at arrival in the specialised office in the Airport of Chisinau City.

For more information, contact Organising Committee of the PMCSC '99, Inst. of Chemistry, Acad. of Sciences of the Republic of Moldova, Academy St. 3, Chisinau MD-2028, R. Moldova, E-mail: garbalau@cc.acad.md, FAX: 373 2 739 954, http://www.asm.md/events/conf99/

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Meeting Calendar

A selection of future meetings. Extensive lists appear regularly in *J. Applied Crystallography*, the *BCA Newsletter* and the *ACA Newsletter* and on the web at http://www.iucr.org/cww-top/mtg.date.html and mirror sites. Corrections and new listings are invited by the Editor.

AUGUST 1999

1-3 ♦ Structure and Dynamics of Molecular and Ionic Solids using Neutrons. Oxford, UK. Contact C.J. Carlile; c.j.carlile@rl.ac.uk.

1-6 ♦ Eleventh American Conf. on Crystal Growth & Epitaxy (ACCGE-11). Tucson, AZ, USA. Contact: T. Gentile, ACCGE-11 Sec., PO Box 3233, Thousand Oaks, CA 91359-0233 USA, FAX: 805 492 4062, aacg@lafn.org; www.aml.arizona.edu/aacg.

2-6 ♦ Denver X-Ray Conf. Steamboat Springs, Colorado, USA. Contact: http://www.dxcicdd.com.

4-13 ♦ 18th IUCr General Assembly and Int'l Congress of Crystallography. Glasgow, Scotland. Contact: www.chem.gla.ac.uk/iucr99/.

16-27 ♦ National School on Neutron and X-ray Scattering. Argonne, IL USA. Contact: nxschool@dep.anl.gov, http://www.dep.anl.gov/nx/index.html.

23-26 ♦ Alfred Benzon Sym. No. 46, Molecular Mechanisms of Innate Immunity. Copenhagen, Denmark. Contact: B. Dalgaard, FAX: 45 3962 0933, benzon@ post1.tele.dk; www.benzon-symposia.dk.

29-3 ♦ 7th Int'l Conf on Ferroelectric Liquid Crystals (FLC 99). Darmstadt U. of Tech., Germany. Contact W. Hasse, FAX 49 61 51 16 49 24; flc99@tu-darmstadt.de; http://flc99.tu-darmstadt.de.

SEPTEMBER 1999

12-17 ♦ Sixth Int'l Conference on Surface X-ray and Neutron Scattering (6SXNS). Noordwijkerhout, The Netherlands. Contact: 6SXNS Sec., FAX: 31 40 2745002, mfrankn@natlab.research.philips.com,

28-30 ♦ Fifth European Conference on Residual Stresses (ECRS5). Noordwijkerhout, The Netherlands. Contact: Conf. Sec. G. van Galen, Netherlands Soc. For Materials Science, P.O. Box 390, NL-3330 AJ Zwijndrecht, The Netherlands, FAX: 31 78 6195735; bvm@worldonline.nl; http://ECRS55.stm.tudelft.nl.

NOVEMBER 1999

3 ♦ PCG Autumn Meeting "Pushing the Limits of Powder Diffraction". CLRC Rutherford Appleton Lab, UK. Contact: C.C. Wilson, FAX: 01235 445720, C.C.Wilson@rl.ac.uk, www.isis.rl.ac.uk/Crystallography/Pushing99.htm.