

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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LETTER FROM THE PRESIDENT

Letter from the President



Henk Schenk

This time a selection from my diary:

Thursday 1 August. In the air on my way to the XIX General Assembly and Congress of the IUCr in Geneva. I realize myself that I have just two more weeks as president. I enjoyed it a lot, but it is good that there is an end as well, it is a time-eater. Tomorrow the six day meeting of the Executive Committee starts and I'm looking forward to that. The EC is a very interesting group of people from all over the world and from all directions in crystallography. This results in intelligent discussions to form opinions and to reach decisions in consensus. Mike Dacombe, our executive secretary, organises a welcome dinner. Most of us are there, a meeting of friends, personal news, recent science, union activities. Time flies, bedtime.

Friday 2 August. I open the EC meeting at 9.00. A long discussion about the finances. In the last triennium we invested a lot, particularly in the new International Tables, in Journals-Online and in JSR. Red figures were the result. However, as sales of the IT are starting and cost reductions are achieved, we are now neutral again and are expecting a better next year. The Journals: Sine Larsen knows the Science Citation impact figures. They are very good, JAC is first out of 19 in the crystallography section, *Acta D* second, *Acta B* fourth and *Acta A* fifth. JSR is third out of 48 in the section Instrumentation. We will introduce an electronic only subscription for retired people. Access to all journals for a small price. Ideal for an emeritus to keep up with science, for the IUCr an increased readership. I'm dining downtown with Ze Zhang. We have a very nice evening with lots of interesting discussions. Tasty fish from the lake and an unexpected second serving. As dessert the splendid fireworks of the Geneva Festival at the lake side.

Saturday 3 August. Many small items today and a preview of all commissions and their reports. But also the International Tables. After all years of preparations five are out now and the remaining four will be out next year. We are very pleased with the sales, the community loves the IT's. The Bio-volume F appears to be a new hit. Spending the evening downtown with many of the group. Dining in a patio. Excellent timing, our meeting and the festival.

Monday 5 August. Today and tomorrow we speak with most of the chairs of commissions and committees. It is fantastic how much these groups of volunteers achieve in favour of crystallography and our Union. And so many initiatives in the planning. Have dinner with Leonid Aslanov to discuss our joint research on pigments on old paintings.

Tuesday 6 August. Opening ceremony of the XIXth congress, downtown Geneva. Three speeches, Joel Bernstein to welcome, Menahem Kaftory to introduce the program and me to open the congress. Then a lively musical intermezzo by a local Klezmer group. I read the text of the certificate of the Ewald prize and vice president Michiyoshi Tanaka presents the beautiful Ewald medal to Michael Woolfson. Photographs. After receiving the certificate, Michael delivered the Ewald lecture. A fascinating talk of a gifted researcher and teacher. Unforgettable. A fantastic reception follows, delicious food, fine wines, great view over Lake Geneva. Meet many of my friends and many young scientists. Make my compliments to Joel Bernstein for this excellent congress start.

Henk Schenk

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EDITORIAL

Editorial



A summary report on the last three volumes of the Newsletter was presented to the Executive Committee at the XII Congress and General Assembly in Geneva. The review reflected how diverse the field of crystallographic research is and how well the newsletter has come to reflect its international scope.

Highlights of the twelve issues published during the 1999-2001 triennium included extensive coverage of the XVIII Congress and General Assembly in Glasgow, preliminary information concerning the XIX Congress in Geneva, cover stories on the 50th anniversary celebration of the IUCr held at the annual meeting of the three regional associates, the publication *Crystallography Across the Sciences*, a collection of review articles based upon the 50th anniversary symposia, the development of online IUCr journals including the new all electronic *Acta Cryst E*, *Structure Reports*, special issues on women in crystallography, dedicated to Dorothy Hodgkin, on the role of crystallography in proteomics, and on the explosive growth of the Protein Data Bank.

Reports of 73 meetings on crystallographic topics in 27 countries were published. Twenty-one of these meetings were general in nature and covered a range of crystallographic topics. The 46 on specific topics concerned materials, powder diffraction, synchrotron applications, hydrogen bonding, chemical crystallography, electron diffraction, electron densities, crystal growth, engineering and chemistry, software, data collection, supramolecular structure, surfaces, strain, molecular biology and drug design.

With the assistance of Andrea Sharpe summaries of selected papers from current IUCr Journals became a regular feature in the newsletter. Twenty-three pages were devoted to summaries of 31 Papers.

Cover illustrations in the 1999-2001 triennium period included examples of small molecule crystallography, macromolecular structures, polymorphism, electron densities, and Geneva meeting sites. Sadly, obituaries of 24 prominent crystallographers were included in the issues of this triennium.

Each issue also contained a letter from the President, news of IUCr Commission activities, notices of elections, awards to crystallographers, and information on books, web sites, resources, and activities of interest to crystallographers. Contributions from crystallographers everywhere were sought, material was gathered from newsletters of crystallographic associations and societies and from leading science news magazines. Reports were received from national crystallographic associations in Australia, Belgium, France, Germany, Israel, Japan, Mexico, Morocco, The Netherlands, Poland, Russia, Serbia, Switzerland, US, UK, and Turkey. Photos were provided by contributors or drawn from the personal collection of the editor. Almost all submitted contributions were published and all material was edited to varying degrees.

The staff of the editorial office in Buffalo, NY, is responsible for desktop preparation of all copy, all negotiations with the printer, postal authorities, and distribution houses, correspondence with contributors, maintenance and production of the mailing list, and solicitation and handling of all advertising.

LETTER TO THE EDITOR

Typographic validation

Dear Bill,

I know you had to precis some of my report on the Symposium in Poznan [*Crystallography in a Castle* (Vol. 9 [4] p. 12, 2001)] but the final version had introduced into it over 30 typographical errors – most of them would be spotted readily by any English-speaking chemical-crystallographer proof-reader. Recalling how much effort I have spent correcting other people's English, etc., I felt it rather ironic that my piece should be so mangled. I realize that editing is a big job and only a fraction of your responsibilities, but the number of errors almost justifies a note of regret in the next issue (I don't know whether any other reports fared as badly). I attended the UK RSC* (not RS) Landmark event at Oxford in May 2001 [*Hodgkon Laboratory* (Vol. 9 [3] p. 11, 2001)]. Although this event in the University Museum was celebrated with wine, I didn't notice any low-flying Hodgkons.

Derry Jones, Royal Society of Chemistry

Dear Derry,

I am sorry about mangling your text so badly. I think we may have achieved an all time high for errors on a single page. At least I hope we don't get much worse. I have a couple of proof readers who usually catch most of my errors. I would like to attribute it to the fact that we have been so far behind and rushing to catch up.

Bill

LETTER TO THE EDITOR

Newsletters online

Dear Dr. Duax,

I have in my hands the *IUCr Newsletter* 9/4. At page 4 ('Editorial') you state, 'The newsletter is placed on the web when it is sent to the printer. You can view it weeks before your hard copy arrives at www.hwi.buffalo.edu/iucr/.' Actually, the 'most recent' issue of the newsletter on that server is 9/2. It's not 'weeks before', it's rather 'several months after'. Perhaps you may wish to update the server, or correct the above statement in the next Editorial.

Massimo Nespolo

Dear Massimo,

We're working on that.

Bill

LETTER TO THE EDITOR

Corrections to the record

To the Editor,

I was rather surprised to find an article written by me in the recent *IUCr Newsletter*, 10,1. After my initial satisfaction that my article was worth republishing in your journal, I found some annoying errors in the text. First of all there was no mention of the fact that this article, under the heading 'Thirty Five Years Ago', was originally published in a special issue of the newsletter of the Commission on Powder Diffraction (No. 26, December 2001), mainly dedicated to the Rietveld method. Secondly you replaced the heading of this article by 'Reitveld on Reitveld'. In itself a felicitous phrase, if not for the fact that by now one should know that my name is written as RIETVELD instead of Reitveld. Finally at the end of the article you made an awkward mistake by writing 'Receiving the Gregori Aminoff Prize gave me added luster' instead of 'Receiving the Gregori Aminoff Prize gave an added luster'. Really I am not that arrogant!

Hugo Rietveld

Dear Hugo,

I apologize for the errors, especially for misspelling your name. I am notoriously bad at spelling and punctuation which should raise questions of how I came to be an editor of anything. Since the rest of the community will note the erroneous spelling of your name, I expect more letters of correction. The substitution of 'me' for 'an' was most unfortunate. Its clear that your luster preceded the Aminoff prize. We try to get attributions properly recorded, but as your letter demonstrates, we have been known to fail. Please accept my sincere apology.

Bill

LETTER TO THE EDITOR

More corrections

Dear Editor

I just received my latest IUCr Newsletter (Vol 10, No. 1) yesterday and was horrified to see the misspelling of Rietveld (Reitveld twice) in the heading to Hugo Rietveld's article on Page 26! My recollection was that this is a not uncommon error amongst authors but interrogation of the Web of Science database for citations to the classic *J. Appl. Crystallogr.* paper gives 3288 citations to Rietveld and a mere 30 to Reitveld.

I have also just noticed on line 3 of the article - 'urinates' - presumably 'uranates' or is someone 'taking the p..s'??

Mike Henderson

Dear Mike,

As errors go, the misspelling of uranates may be the 'piece de résistance'.

Bill

Crystallographic databases

A Joint Special Issue of *Acta Crystallographica Sections B and D*



In April 2002, the five crystallographic structural databases recorded a total of 407,979 crystal structures derived principally from published papers. Release 2001 of the Powder Diffraction File contained details of 136,895 powder patterns. All of the databases offer software systems for search, visualization and data analysis that continue to make best use of state-of-the-art computing and communications technology.

Most importantly, these databases and software resources are now part of the infrastructure of science, and are used all over the world by a wide spectrum of physical, chemical and biological scientists who have an interest in the spatial structure of chemical compounds. They answer questions that range from the simple but essential library functions to complex queries on three-dimensional structural systematics. Knowledge derived from them is used in applications programs that contribute to wide-ranging developments in industry and academia. The number of published applications of the crystallographic databases now runs well into four figures.

The joint special issue of *Acta Crystallographica Sections B and D* of June 2002 presents an in-depth survey of the current status of the crystallographic databases, their software resources and, most importantly, their scientific applications. The 18 papers (146 pages in total) cover areas ranging from computational materials design to protein-protein interactions, protein dynamics and protein modelling. In between are examples of the value of existing structural knowledge, e.g., in the identification of unknowns, as an aid in solving novel structures from powder diffraction data, in the study and classification of molecular conformations, and in the systematic study and categorization of intermolecular interactions. The special issue shows how knowledge bases can be derived from databases, and how that knowledge is often crucial in the life sciences, particularly in the *de novo* design of novel pharmaceuticals.

The issue celebrates the richness of fundamental information established by crystal structure analysis. It shows that each and every structure has a value that transcends the original purpose of the study. As more and more crystal structures lie dormant in computer files across the world, we should reflect on the information loss that is entailed, and work to ensure that *all* of these incomparable information sources are captured for use by current and future generations of scientists.

The special issue comprises pages that form parts of Volumes B58 and D58 of *Acta Crystallographica*. It is also available as a complete and comprehensive single volume for individual purchase at a price of US\$30/EUR35 per copy.

Frank Allen, Cambridge Crystallographic Data Centre, UK

MEETING REPORT

ECM20

August 25-31, 2001

[Continued from Volume 10 number1]

The emphasis in the microsymposium 'Polymorphism and Solid State Chemistry' was on inorganic systems.

The microsymposium was organized jointly by the 'Mineralogical Crystallography' (SIG5) and the 'Molecular Interaction and Recognition' (SIG7) SIG's of the ECA.

M. Nespolo (NIMS-AML, Japan) reviewed the IUCr definition of polytypism and pointed out its shortcomings, a lack of geometricity and overemphasis on the chemical aspects, rather than structural features. Polytypes are defined in terms of building layers with a partly idealized geometry (layer archetypes) and symmetry operations relating pairs of layers. Chemical composition differentiates the various families of polytypes.

E.L. Belokoneva (Moscow U., Russia), discussed the inter-transformations among the polymorphs in the LnBGeO_5 ($\text{Ln} = \text{La} - \text{Er}$) family of borogermanates, showing that the structure is analogous to datolite for $\text{Ln} = \text{Nd-Er}$ and to stillwellites for $\text{Ln} = \text{La-Pr}$. The phase transformation from the polar $P3_1$ space-group type to the non-polar $P3_12_1$ space-group type could be described as a complex movement of the B-O tetrahedra along the 3_1 polar axis having both displacive and order-disorder character.

J. Hybler (Czech Academy of Sciences, Praha) discussed 'Cronstedtite polymorphism - an X-ray and HRTEM study' showing the first experimental occurrence of intergrowth of polytypes belonging to different OD subfamilies in this group of 1:1 layer silicates. In some of the pyramidal crystals investigated, the proportion of different subfamilies varies with the location inside the sample, with intergrowth in the central part, and separation of the subfamilies in the external parts.

M. Ellner (Max Planck Inst. for Metal Research, Germany) discussed the mechanism of transformation from the interstitial solid solution Pd(B) , which forms above 723K, to Pd_5B , which occurs at 658K. The atomic radius ratio for B and Pd is 0.71 and, according to Hagg's rule, it is too high for the formation of an interstitial solid solution. The hard-sphere model cannot explain its occurrence. Pd_5B is the Pd-richest boride phase of the Pd-B system and is based on a sub cell of the Pd(B) phase.

M. Hostettler (U. de Lausanne, Switzerland) discussed three polymorphs of 'Mercuric Iodide' that crystallize concomitantly. In a lovely series of carefully controlled experiments he also observed that the three phases could be obtained in stages, from least stable to most stable. Of particular interest is the intermediate metastable phase, whose complex structure comprises two MDO (Maximum Degree of

Order) OD polytypes. The stable phase differs from the intermediate phase only in the distribution of Hg, but the nearest-neighbor coordination is preserved.

Joel Bernstein and Massimo Nespolo

MEETING REPORT

Radiation damage workshop

Chicago, IL USA - December 1 - 2, 2001



Participants at the Third Int'l Workshop on Radiation Damage to Crystalline Biological Samples, December 1-2, 2001. (Photo by Martin Weik)

The Second Int'l Workshop on Radiation Damage to Crystalline Samples was held at the APS, Chicago, December 1-2, 2001. There were 17 presentations and 49 participants who engaged in lively and extensive discussion throughout the Workshop. Topics included: experiences of data collection at very high intensities, radiation damage at specific sites in a protein, effect of damage on structure determination by MAD and SAD, modelling of putative heating effects at high intensities, experience of the use of helium for cryo-cooling, and the assessment of the onset of increasing degrees of radiation damage as a function of dose and dose rate.

There was a protracted debate on the best radiation damage indicators. Further questions requiring experimental answers were posed and best practice for such systematic studies was discussed. This included the necessity of stating the incident and absorbed doses for all measurements, and the care required in varying only one experimental parameter at a time.

The Workshop was funded by DoE-OBER and NIHNCMR, USA, and organized by E. Garman (Oxford), C. Nave (SRS, Daresbury) and G. Rosenbaum (Georgia). Information can be obtained at www.aps.anl.gov/conferences/damage. Eight papers containing material presented at the workshop will appear in the *Journal of Synchrotron Radiation*, September 2002.

Elsbeth F. Garman

MEETING REPORT

From genes to drugs in Erice 2002

Erice, Sicily, May 2002



The genomics revolution is here – are you ready? Participants at the 33rd Erice course *From Genes to Drugs via Crystallography* directed by N. Borkakoti of Mediver UK Ltd learned that this revolution is having a profound impact on the field of drug design. Genomics provides boundless data regarding sequences and potential drug targets; the challenge for structural scientists will be to extract information and knowledge from the data.



The Emerald Team, the 'Flow Chart' Winners.

How? Some of the answers provided by the speakers at this school are **scale-up** and **high throughput**.

Scale-up to use the mounds of sequence data and the increasing number of known macromolecular structures to predict function, or scale-up to enable the determination of every macromolecular structure coded by a genome, or scale-up to screen every available compound in either a real or virtual database as a target ligand for the development of drugs. High throughput is a familiar concept when it comes to screening potential ligands for a new macromolecular target, whether through biological testing or through docking computations. High throughput has been a requirement for the methods that were developed to analyze the explosion of sequence and structural data in recent years. Now structural genomics groups are developing high throughput and automated technologies for macromolecular structure determination because these groups seek to complete the structural library of a genome. The automated determination of protein structures and the subsequent abundance of structural information will have many implications for our community with regards to the quality of the structures, the methods for extracting meaning from the vast array of structures, and the way macromolecular crystallographic research is done, funded and published; hence the question at the beginning of this article – are we ready?

The 33rd Crystallography Course was held by the Int'l School of Crystallography, Ettore Majorana Foundation and Centre for Scientific Culture in Erice, Sicily, May 23 - June 2, 2002. The program began with a historical review of ideas from H. Hauptman (Buffalo, USA), of crystallographic milestones from J. Glusker (Philadelphia, USA), and of drug design from P. Goodford (Oxford, UK) and then covered the components of the pathway from a target gene through sequence, function and structure determination to identification of ligands and effective drugs, beginning with an overview from T. Blundell (Cambridge, UK), Director of the School.

A major component of the drug design pathway presented at the meeting was structural genomics, which builds on the advances in molecular biology, including multiplex cloning, to study the structures coded in a genome. Many consortia have been established world-wide to address this challenge. The consortia bring together molecular biologists, bioinformatics specialists, crystallographers and others to identify target proteins and produce their structures. Groups are variously organized to develop high throughput technologies, to focus on either functional targets or on characterization of new folds, or to compile the entire structural library of a genome. Both tightly coupled and open collaborative large-scale

structural genomics consortia, as well as single laboratories focused on a specific target function, were represented at the meeting. Presentations outlined the advances in technology for high-throughput cloning and crystallography, techniques for crystallization of membrane proteins, and the contributions of other physical methods: NMR, mass spectroscopy, and cryo-electron microscopy to structural genomics.

Structural genomics projects promise a profusion of structural data that will match the enormity of the sequence database. Bioinformatics scientists are faced with the challenge of decoding the relationships among sequence, structure and function. Advances in prediction of new folds from sequence, function from structure, and function from sequence were presented and opened the question regarding which of structure, function and sequence is the unique determinant. Another feature of the volume of data available is the several thousand protein binding sites tabulated in the PDB; these data allow groups to identify the common features of a 'beautiful binding site' and to seek such sites in new structures generated by the genomics information explosion. These promising methods will be important to the extraction of information from the structural data that will help in the prediction of function from sequence and structure.

Ligand design and screening provided another focus for the course. Speakers covered the many computational approaches to mapping binding sites and screening large libraries of potential drug compounds with docking algorithms that identify novel chemical classes and serve as excellent generators of ideas. Several different computer screening approaches were presented along with examples of successful applications. Difficulties regarding the development of effective scoring functions for ranking hits and the computation of bioavailability (adsorption, distribution, metabolism, and excretion) were reviewed, and the relative value of virtual high throughput screening (HTS) vs. HTS by biological assay was debated. In each case, the goal is the generation of novel starting points for further drug development. Throughout the discussion, the importance of the quality of the crystallographic structural information was highlighted since it is the basis for the development of interaction potentials and scoring functions and for the identification of binding sites.

An exciting set of presentations outlined the results of drug design efforts and the range of macromolecular targets that can be drug targets. High resolution structural work on Factor Xa, lysosomal cysteine proteases and IMP-1 (a metallo- β -lactamase) demonstrated how powerfully crystallographic results can influence the drug design process. Results on large structures – summarized in a mini-symposium on the ribosome and in the description of the inhibition of picornavirus - demonstrated the importance of these large structures in the development of therapeutic agents.

The lecture portion of the course was supported by an excellent set of workshops covering protein crystallization, databases (Cambridge Structural Database, Protein Data Bank), structural checking (WHATCHECK), docking (DOCK, FlexX), bioinformatics, and metal ion geometries. In addition, teams of participants were challenged by the Director to develop flow charts that mapped the pathway between genes and drugs. The flow chart exercise highlighted the complexity of the drug design process; participants used a variety of images - finding a needle in a haystack, wandering the complex street map of the ancient city of Erice (where the Edelweiss Hotel and the Edelweiss Restaurant are not even on the same street!), the ball passing pattern in a football match – as representations of the pathway from genes to drugs. Finally, J. Bernstein's (Beer-Sheva, Israel) presentation regarding the pitfalls of patent law and the risks inherent in testifying as an expert witness added a new dimension to the scientific discussions of designing drugs.

Much of the lecture material presented at the course, as well as the flow charts, will be available on the course website, www.geomin.unibo.it/orgv/erice/downloads.htm. The course was timely, instructive, provocative, and fun thanks to the superb direction of N. Borkakoti and, as always, the outstanding local organization provided by P. Spadon, L. Riva de Sanseverino and their many assistants deserves special mention. Director Borkakoti's program provided a fine summary of the state-of-the-art in drug design and

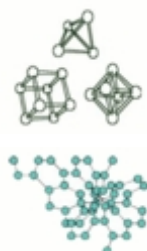
the local organizers made sure that the cultural and scientific activities of the conference were enjoyed by each participant. The crystallographic community is privileged to have access to the fine conference facilities at Erice and truly blessed that Lodovico and Paola are such gifted organizers.

Penny Coddling

MEETING REPORT

Eleventh Slovenian - Croatian meeting

Bohinj, Slovenia, June 2002



Science not only knows no boundaries, but has a way of dissolving them. Sixty-eight crystallographers from seven countries gathered at the 11th Slovenian-Croatian crystallographic meeting.



Plenary lecturers (from left) G. Giester, D. Matkovic-Calogovic, B. Modec, H. Boehm, and E.R.T. Tiekink at the 11th Slovenian-Croatian crystallographic meeting.

There were five plenary lectures 'Phase Transitions In Modulated Structures' (H. Boehm, Germany), 'Five Years Of CCD X-Ray Data Collection At Vienna University' (G. Giester, Austria), 'Adventures In Engineering Molecular Solids' (E.R.T. Tiekink, Singapore), 'Protein Crystallography - A Small Molecule Crystallographer's View' (D. Matkovic-Calogovic, Croatia), 'Oxomolybdenum(V) Clusters Built of Dinuclear Metal-Metal Bonded Units' (B. Modec, Slovenia)], and 40 additional oral presentations including contributions from representatives of Bruker-Nonius, Anton Paar and Mikro-Polo. The short presentations concerned proteins, organic and organometallic structures, inorganic structures, coordination compounds, metallic alloys and oxides, minerals, powder diffraction, microporous material, and zeolites. L. Golic (Ljubljana) and B. Kamenar (Zagreb) began this series of meetings in 1992 after the disintegration of Yugoslavia and maintained their annual organization. The rainy excursion to the vast green forests of Pokljuka, a plateau in the Julian Alps was exceptionally memorable. The crystallographers from Slovenia and Croatia have been gathering now for 11 years.

E. Tillmanns (Vienna, Austria) and E.R.T. Tiekink (Singapore), Co-editors of two crystallographic journals, attended the meeting. The latter is one of the most prolific writers of crystallographic papers (714 papers with 3274 citations, Web of Science, ISI).

In the Closing Remarks, S. Popovic (Zagreb, Croatia) expressed gratitude to the lecturers, the sponsors, and the Organizing Committee and announced that 'In order to match the beauty of the Bohinj Lake in the Triglav Nat'l Park, the excursions at the 12th C-S meeting in June, 2003 will be to Plitvice Lakes Nat'l Park. The park is protected by UNESCO as a world heritage site. The sixteen clear water lakes, water falls with fascinating audio and visual beauty, and the blue-green water enhances the beauty of the green woods. All *bona fide* scientists and their friends are invited to attend the Meeting.' For additional information, contact S. Popovic (Zagreb, Croatia) at spopovic@phy.hr.

Ivan Leban

MEETING REPORT

German Crystallographic Assn (DGK) 10th annual meeting

German Crystallographic Assn (DGK) 10th annual meeting

Kiel, March 2002



The city of Kiel close to the Baltic Sea is well known for numerous national and international sailing activities. The university of this city, the 'Christian-Alberts-U. zu Kiel', hosted this year's DGK meeting held March 4-7, 2002. In addition, a public exhibition on 'Crystals in Art and Science' (see contribution of W. Depmeier below) started in parallel to this meeting. Both events were organized by the Inst. of Geosciences. About 400 participants attended the meeting. The scientific program comprised nine plenary lectures, two parallel series of micro symposia on general crystallography and on structural biology with about 30 contributions each, and in total more than 220 poster presentations, which covered almost all fields related to crystallography.

The topics of the plenary lectures spanned the wide range of interests of the German crystallographic community including 'HTP structural genomics' (U. Heinemann), 'Using high-T and high-P chemistry to synthesize new nitro silicates and nitro phosphates' (W. Schnick), 'Crystal engineering: structure and properties' (G. Desiraju), 'Fundamental studies in clathrate hydrates' (J. Tse), 'Modelling of quasicrystals by a quasi unit cell' (P. Gummelt) and 'Diffraction from polycrystals using synchrotron radiation' (H. Ehrenberg, 2001 Max-von-Laue prize laureate talk).

During the last session of the meeting 'New methods - the future of crystallography' plenary talks were presented on 'The European Spallation Source (ESS) Projects' (D. Richter), 'The DESY X-ray free electron laser: a quick look on atoms' (J.R. Schneider) and 'What can simulators offer crystallographers' (J. Gale). The first two talks presented plans for large science infrastructure projects in Europe. The third talk summarized the present state of computational crystallography. The following discussion embracing the justification of the costs for large scale research facilities was quite lively, but finally most of the participants agreed that scientists should first concentrate on the new scientific opportunities of the planned projects.

The topics of the microsymposia sessions included theory, X-ray diffraction studies, teaching, synchrotron and neutron diffraction, and solid state NMR. Parallel microsymposia on structural biology covered industrial crystallography, methods and instrumentation, new structures, structural genomics and membrane proteins.

For several years now DGK has awarded two prizes during the annual meeting. This year the Max-von-Laue prize for outstanding achievements of young scientists was received by M. Fechtelkord, who made his main contributions in solid state NMR. He will give a plenary lecture on this topic during next year's DGK meeting in Berlin. The second prize, the Carl-Hermann-Medal, is awarded to distinguished crystallographers in order to honour their lifework. This year's Carl-Hermann-Medal was awarded to F. Liebau who made very important contributions to our knowledge about silicates during his scientific career.

The scientific program was accompanied by a social evening event that took place in the 'Kieler Markthalle'.

Edgar Weckert

MEETING REPORT

Crystals in arts and science

Kiel, March, 2002

On the occasion of the 10th Annual Meeting of the German Crystallographic Assn, the DGK, held at the U. of Kiel, March 4 - 7, 2002, an exhibition was organized by two crystallographers, Wulf Depmeier and Horst Küppers and artists V. Eliasberg, B. Manitz and I. Moor from the Muthesius School of Fine Arts. The exhibition 'Corners & Edges - The Crystal in Science and Arts' which took place at the Kieler Stadtmuseum Warleberger Hof stimulated a dialogue among scientists and artists as to why people are fascinated by crystals.

One focus of the exhibition was on expressionist painters Hans Scharoun, Bruno Taut, Wassili Luckardt, Wenzel Hablik and F. Peter Droemmer who depict crystals in a more or less metaphorical way. A few natural mineral specimens helped to illustrate the artists' fascination with crystals.

The spatial illusions of Hermann Paulsen, Susanne Dölker's humorous zeolite framework, the sensitive paintings of Valeria Eliasberg and Irina Moor, the elegant textile objects of the group XX-TeX organised by Annegret Haake, the impressive Euclidean space tilings of Friedhelm Kürpig, and the magic models of minimal surfaces of the crystallographer Elke Koch, made a deep impression on the viewers. The figure shows V. Eliasberg's painting 'Der Raum' ('Space').

Of particular interest to crystallographers was the life work of crystallographer mathematician Heinrich Heesch Kiel. His work on plane tilings, black-and-white groups and the four-colour problem was represented with several exhibits. Other exhibits concerned the expressionist painter F. Peter Droemmer of Kiel and the history of the Mineralogical Inst.

About 3000 visitors attended the exhibition over 30 days. The exhibit catalogue described the history of the Mineralogy/Crystallography Inst. in Kiel. A virtual tour of the exhibition, which is also available on CD, can be found on the website www.ifg.uni-kiel.de/eckenundkanten/.

The exhibition would not have been possible without the generous sponsorship of the DGK and the IUCr.

W. Depmeier

MEETING REPORT

Highlights of ACA 2002

San Antonio, TX - May 2002



Electron microscopists

The San Antonio meeting featured symposia on electron diffraction crystallography and electron microscopy occasioned by the presentation of the Patterson award to D. Dorset and an ACA Transactions Symposium on powder diffraction, organized by A. Clearfield. The symposia reflect the multidisciplinary ACA mission to support all investigations into the structure of matter and brought many new faces to the meeting. The electron microscopists and powder diffractionists are mounting efforts to found new ACA SIGs.

At the Awards banquet, Wood Scientific Writing Award winner Ira Flatow regaled us with a spirited description of the role of experimentation in developing his inimitable journalistic style.



Powder diffractionists

Latin American scientists attending the meeting explored ways that the ACA, as an IUCr regional affiliate, could help strengthen crystallography in Latin America. Signatures are being solicited from current ACA members in Latin America to form a new SIG, and a new fund has been established, the assets of which will help advance the Latin American initiative, and provide partial support for Latin American students to attend future ACA meetings.



Electron diffractionists

Five applications from groups offering to host future ACA Summer schools were reviewed. In 2003 the ACA will support a course in small molecule fundamentals at Indiana U. of Pennsylvania, and a more extensive course, primarily centered on macromolecular crystallography, at the Illinois Inst. of Technology in Chicago.



Latin American crystallographers with ACA council members

In San Antonio, the recent explosive growth of corporate crystallography produced a challenge to our scientific and intellectual health. Industry-based speakers invited to discuss their work were replaced by 'company' personnel because the invited speakers were no longer associated with a particular company. Platform and informal discussions were compromised by constraints arising from threatened hostile legal action based on what many found to be a miscarriage of patent law. While admitting that much remains to be learned, these examples represent new and highly unwelcome pathologies that threaten to disrupt broad aspects of scientific exchange. It is essential that we minimize the very real threat of intellectual nuclear winter.

Charlie Carter

FEATURE ARTICLE

Convergent-beam electron diffraction

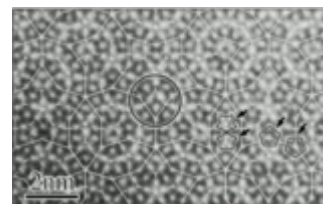


'Beauty under blossoms' (T. Ishikawa)

The cover illustration is taken from a new book by Michiyoshi Tanaka and collaborators on electron diffraction. The book is not only scientifically sound and comprehensive, but it is visually stunning. Excerpts from the introduction and a sample of the wonderful illustrations are reprinted here – W. L. Duax, Editor

The convergent-beam electron diffraction (CBED) method is well-established in electron microscopy as an important analytical technique for the study of materials. The CBED method is widely used in materials science research for symmetry determination and strain measurements of multi-layers.

Coherent CBED, which uses a highly coherent electron source (i.e. a field-emission gun), is also a method of directly providing phase information on crystal structure factors. The coherent CBED technique produces interference fringes in the overlapping regions of CBED disks. From the relative positions of the fringes, the phase differences between two diffraction waves can be determined. The coherent CBED method can distinguish 12 space-group pairs among the 23 indistinguishable sets, and provides full dynamical methods to refine crystal structure parameters.



Since 1990, our major objective has been to develop a high-precision crystal structure refinement method based on the full dynamical theory of electron microscopy, which enables energy filtering of a CBED pattern containing both zero order Laue zone (ZOLZ) and higher order Laue zone (HOLZ) reflections. With support from JEOL and the Ministry of Education, Science, Sports and Culture of Japan, we manufactured an electron microscope (JEM- 2010FEF) equipped with a field emission gun, an objective lens with a small Cs and an omega filter. In this volume we describe examples of energy-filtered CBED patterns, a new spacegroup determination method which uses the coherent CBED technique, case studies of crystal structure refinements of CdS, LaCrO_3 and h-BaTiO_3 including charge density determination, simulations of Kikuchi patterns due to thermal diffuse scattering, recent studies of quasicrystals, interface analysis, which is an important application to device technology, and a future trend of the electron microscopy, an atlas of CBED symmetries for handy reference and CBED pictures for the reader's enjoyment. The photographs were taken with JEOL electron scopes JEM-2010 and JEM-2010FEF using an imaging plate system.

Michiyoshi Tanaka, Sendai, Spring 2002

NOTICE

What is crystallography?



What is crystallography? This is the question recently posed by Walter Steurer, Editor in Chief of *Zeitschrift für Kristallographie*, in an invitation to crystallographers worldwide to contribute to a special issue of *Zeitschrift für Kristallographie* on the occasion of its 125th anniversary. This special issue will contain short contributions of 125 crystallographers and a summary of their personal opinions. To quote Prof. Steurer: 'There is an ongoing discussion at many universities if crystallographic research and teaching is still timely. In many cases retired professors of crystallography are not being replaced by crystallographers any more. One of the reasons for this development may be that crystallography is commonly seen in its narrow definition as a method for routine structure analysis.

In my opinion, there has opened a wide gap between the self-understanding of the crystallographic community and the perception from outside. At the triennial conferences of the IUCr it is shown what modern crystallography comprises. I believe, however, that most of the participants would not call themselves crystallographers despite the fact that they do excellent crystallographic research.

This may be related to the fact that it is not clear whether crystallography is a scientific discipline or just a suite of methods. R.W. Cahn, in his book 'The coming of Materials Science' (Pergamon 2001), calls crystallography an exceptional *parepisteme*, i.e. a kind of subsidiary topic or subdiscipline. Disciplines are degree subjects at universities while *parepistemes* such as crystallography usually form components of degree courses only.

Anyway, modern crystallography is a dynamic and innovative interdisciplinary structural science. This should be better communicated to the scientific community, the science administration, the funding agencies and the politicians. The planned special issue of *Zeitschrift für Kristallographie* is to contribute to this process.' To provoke discussion about what modern crystallography involves, Prof. Steurer sought comments on the following:

1. What is crystallography? Give your personal definition.
2. Is there a better name that could replace the historical term crystallography'?
3. What are the most important unsolved problems in crystallography? Give your personal list.
4. What is the future of crystallography?
5. Should we still teach crystallography? Why and how should we teach?
6. Personal recommendation to a student who wants to enter into crystallographic research.
7. What is the impact of crystallographic research? What would you tell your funding agency or the president of your university? What would you tell the taxpayer?

All members of crystallographic associations worldwide (ACA, BCA, SCANZ, ECA, AsCA etc.) should take these questions to heart and contemplate how they would respond. I look forward to reading the special issue [August 2002].

*Mark Spackman, President, Soc. of Crystallography in Australia and New Zealand
from SCANZ Newsletter, No. 52, May 2002*

AWARDS AND PRIZES

New medal named for Rosalind Franklin

The UK is honoring crystallographer Rosalind Franklin (1920-1958) by creating a medal in her name to recognize innovations in science. Franklin's research was largely ignored during her lifetime, but is now widely accepted as having been key to discovering the structure of DNA. The new medal – the Royal Society's first to carry a woman's name – has a purse worth £30,000 (approximately \$42,000).

Franklin died four years before the Nobel Prize in Medicine went to Francis H. C. Crick, James D. Watson, and Maurice H. F. Wilkins for the discovery of the structure of DNA.

The new medal, which will be presented annually, is open to all UK researchers, male and female. It has one of the largest monetary values of any UK award.

Details can be found on the Royal Society Website at www.royalsoc.ac.uk. The inaugural medal will be bestowed next year to coincide with the 50th Anniversary of the publication of Crick and Watson's *Nature* article on DNA.

Paul Guinnessy

AWARDS AND PRIZES

American Crystallographic Association awards

Winners of Warren and Buerger Awards



During the ACA meeting in San Antonio the selection committee (P. Butler, chair, J. Johnson, I. Robinson, and B. Stec) announced that the 2003 Bertram E. Warren Diffraction Physics Award will be presented to **Takeshi Egami** (U. of Pennsylvania) and the selection committee (J. Kaduk, chair, R. Blessing, G. Bricogne and S. Doublié) announced that the 2003 Martin J. Buerger Award will be presented to **James Ibers** (Northwestern U.).

The awards will be presented at the ACA meeting in Greater Cincinnati (Northern KY) in July 2003. Symposia will be planned around the winners of the two awards.

ACA Peggy Etter Awards

In recent years, the ACA has provided student travel support through awards named after the late Peggy Etter. At the ACA Council Meeting in San Antonio, a decision was taken to formally implement two separate awards named after Peggy Etter that recognize her scientific accomplishments and her reputation as an outstanding mentor of students and junior colleagues. The Margaret C. Etter Early Career Award will recognize achievement and future potential among those at an early stage in their independent careers. The citation for the award and the guidelines for submitting nominations are available on the ACA web site. The Margaret C. Etter Student Lecturer Award will be presented to a small group of students each year who have been selected to give oral presentations at the ACA meeting. The award will be entirely independent of the ACA travel awards, which will remain open to students, postdoctorals and young scientists.

For further information visit www.hwi.buffalo.edu/aca/

Lee Brammer, ACA Secretary

REGIONAL NEWS

American Association for Crystal Growth elections

www.crystalgrowth.org/



Executive Committee elected to six year terms: E. Bourret-Courchesne, J. Derby, D. Kaiser, D.

Matthiesen, R. Scripa, R. Sekerka, G. Stringfellow, F. Szofran, D. Vanderwater, C. Wang, and M. Wargo.

Returning elected members: T. Kuech (President), P. Morris-Hotsenpiller (Vice President), D. Bliss

(Treasurer), E. Monberg (Secretary), D. Brandle (Past President 1993-96), V. Fratello (Past President 1996

-99), L. Boatner, J. DeYoreo, M. DiGiuseppe, K. Jackson, Gabe Loiacono, Stu Samuelson, N.B. Singh, T.

Surek, W. Wilcox, and G. Witt.

REGIONAL NEWS

New X-ray facility

A new Centre called the Integrated Victorian X-Ray Structural Determination and Materials Characterisation Facility has been set up in Victoria from an ARC REIF grant. This facility involves collaboration between the U. of Melbourne, RMIT, LaTrobe U., the Australian Radiation Protection and Nuclear Safety Agency (ARPNSA) and the Victorian U. of Technology.

The Chief investigators are: Jonathan White (Melbourne U.), Suresh Barghava and Kay Latham (RMIT), John Orbell (Victoria U. of Technology), Geoff Williams (ARPNSA), and Andrew Hughes (LaTrobe).

from SCANZ Newsletter, No. 52, May 2002

AWARDS AND PRIZES

Congratulations...

John W. Cahn, senior fellow at the Nat'l Inst. of Standards & Technology (US), received the Bower Award & Prize for Achievement in Science for his accomplishments in the understanding of the thermodynamics and kinetics of phase transformations. His dedication to understanding materials has inspired scientists and engineers and led directly to the creation of multifunctional materials based on his ground-breaking theories.

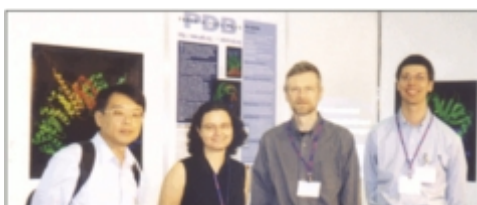
Jennifer A. Doudna, Professor of Biochemistry & Molecular Biology (U. of California, Berkeley), was elected to membership in the US Nat'l Academy of Science.

NOTICE

Biological databases



In structural biology we have one of the oldest established biological databases, the Protein Data Bank. Incredibly it was effectively established in 1971 when only a handful of atomic resolution crystals had been solved. What catalyzed its formation were advances in computer graphics, which, despite having no more than 32k of CPU memory to work with, allowed molecules of the size of proteins to be displayed relatively easily. For the graphic programs to work effectively across the entire database, the files needed to be in a standard format, including such basic concerns as whether the coordinates were measured in centimeters or inches. With the establishment of the PDB it was possible to look at any of the known protein structures in the same way.



Masami Kusunoki, Kyle Burkhardt, Bohdan Schneider, and Wolfgang Bluhm at the PDB booth at the IUCr meeting.

The PDB moved from a centralized location at the Brookhaven National Lab to a consortium encompassing three sites. The content has increased from a few structures to well in excess of 15,000 today, and is on course to have ~45,000 entries by 2005. The completeness of the PDB has been assured by the policy of journals, including *Nature Structural Biology*, to demand that structures cannot be published in their pages without simultaneous deposition. The accuracy of the database is policed by suites of checking programs to detect errors in coordinates when they are submitted.

There is much to be gained by establishing compatible formats and ontology across a range of databases. With compatibility, pieces of software called 'intelligent agents' will be able to extract related information from any and all databases in which it may reside. Such standardization would almost abolish the need for databases to be comprehensive because data would be available from more than one source. Comparing information gleaned from several sources could provide an assessment of the accuracy of those data. By standardizing the way atomic coordinates are documented, the PDB has proven an invaluable boon to structural biology. How much more useful to bioinformatics, in all its guises, would be standardization of the databases themselves?

Nature Structural Biology, Vol. 9, No. 7, July 2002

NOTICE

Beamlines



The prioritization process for the third tranche of beamlines is starting now, to be available in 2008.

Outline proposals for new beamlines are invited from the scientific community and from non-UK government and commercial organizations. The proposals can be for beamlines on insertion devices or bending magnets. Outlines should be no more than three sides of A4 and include: the science case; an outline specification of the beamline; and a summary of the community that would make use of the beamline. The deadline is November 1, 2002. Proposals submitted last year may be resubmitted.

A selection will be made and the successful proposers will be invited to submit a more detailed specification and costing by March 2003. Final selection of up to four beamlines will be made after May 2003.

Further information is available at www.diamond.ac.uk/.

NOTICE

Crystallography web watch

The ACA Communications Committee continues its 'Web Watch' in an attempt to keep members informed of useful websites, primarily of the crystallographic persuasion.

Collaborative Computational Projects (CCPs) — The goals of these British-funded projects are to develop, maintain and distribute computer programs and to promote the best research computational methods in biology, chemistry, physics and engineering. Sites of particular interest to crystallographers: CCP4 (protein crystallography): www.ccp4.ac.uk/main.html, CCP13 (fiber, polymer diffraction): www.ccp13.ac.uk/ and CCP14 (powder, small molecule single crystal diffraction): www.ccp14.ac.uk/index.html.

Linux for Crystallography — The number of crystallographic programs that run under the Linux operating system is rapidly expanding. Look for programs currently available at zeus.polsl.gliwice.pl/~nikodem/linux4chemistry.html, www.ccp4.ac.uk/newsletter36/11_linux.html, or, www.fos.su.se/struc/linux/linuxtal.html.

Crystallographic Software — Network Science has a site that lists crystallographic software from A-Z: www.netsci.org/Resources/Software/Struct/xray.html.

ChemSoc — The Royal Soc. of Chemistry's chemical science network contains considerable information, including a visual interpretation of the periodic table, a timeline of events in chemical history, access to conference and society information, IUPAC draft recommendations, career information, and a listing of web links to a variety of databases: www.chemsoc.org.

Macromolecular Crystallization — Two nice websites are T. Bergfors' Pictorial library of crystallization drop phenomena: xray.bmc.uu.se/~terese/crystallization/library.html and J. Zeelen's X-tal protocols: www.mpibp-frankfurt.mpg.de/~johan.zeelen//xtal.html.

Frank Rotella

OBITUARY

Ronald Jenkins (1932-2002)

Dr. Jenkins, born in 1932 in Oxford, England, died peacefully on June 19, 2002 of prostate cancer at his home in Downingtown, PA. A Celebration of Life service was held at the West Chester Church of the Nazarene, West Chester, PA, June 22, 2002.

Dr. Jenkins studied Chemical Physics at Oxford Polytechnic Inst. in England and obtained his Ph.D. from Polytechnic Inst. of New York. He was a Licentiate of the Royal Inst. of Chemistry, a Fellow and Chartered Physicist of the Inst. of Physics, a Distinguished Fellow of the Int'l Centre for Diffraction Data (ICDD) and an Honorary Member of the British Crystallographic Assn.

Dr. Jenkins worked as an analytical chemist at Esso Research in Abingdon, England, and later as head of the X-ray Applications Lab for Philips Electronics in the Netherlands. He was transferred to the US in 1971 and became the Principal Scientist for Philips Electronics Instruments. In 1985 he accepted the position of Principal Scientist with the ICDD and in 1996 was appointed its Executive Director.

Dr. Jenkins was well known around the world for his contributions in the X-ray analytical science fields of spectrometry and diffractometry. He wrote 4 widely used text books on these subjects, 11 book chapters, and published about 230 scientific papers. He taught these subjects around the world to an estimated 5000 students, organized scientific meetings, including the Denver X-ray Conference for 30 years, established the *International Journal of X-Ray Spectrometry*, and received numerous awards and recognition for his work, including the Birks Award for X-ray Spectrometry and the Barrett Award for X-ray Diffraction, the only person to ever win both awards.

In addition to his technical achievements, Dr. Jenkins was a member of STURP (Shroud of Turin Research Project) and lectured over 50 times to about 6000 people regarding the artifact. His book *Closing the Gap between Science and Religion* outlines his dedication to the Christian faith. He was most recently a member of the Church of the Nazarene, where he served as Council member and Choir Director. He was also a trustee of Eastern Nazarene College in Quincy, MA, USA for many years.

Dr. Jenkins is survived by his wife of 47 years, Phyllis, five children and five grandchildren. Instead of flowers, the family requests that donations be given to the American Cancer Society.

International Center for Diffraction Data

OBITUARY

Bob Cheary (1947-2002)

Bob Cheary, a member of the Applied Physics Dept at UTS for almost 30 years, died February 1, 2002 in Sydney, Australia, at age 55. A great teacher, researcher and above all a man with the ability to communicate warmly and with interest to students, colleagues and administrators, Bob is sadly missed by all those who had the privilege to know him. After a practical background in hospitals and electric research laboratories in England, Bob graduated in Mathematical Physics in 1968 and completed his PhD in 'X-Ray Diffraction Line Broadening in Magnetic Oxides' at Aston U., Birmingham, UK. He joined NSWIT in 1972 and became an active participant in the development of the Applied Physics Degree Course. Bob was keen to strengthen the practical components of the course. When a student once enquired about Bob's apparent career change from mathematical physics to experimental physics using x-rays, he said 'I got too lonely doing theoretical physics. I like to have people around'. People liked to be around Bob too. As Head of Dept of Applied Physics in 1991 Bob led a revitalization of the Physics Laboratory Teaching Program, based on his industrial experiences and commitment to the value of practical hands-on training for students. With his enthusiasm for the applicability of physics to all areas of modern living Bob had valuable associations with colleagues in engineering, and the biological sciences. He worked with the Mechanical Engineering staff to prepare a hands-on based course in Electrical Machinery and with Electrical Engineering staff to develop student-orientated ways of teaching electronics. He disdained honors, but when the department nominated him for the Inaugural Faculty Excellence in Teaching Award, past students and associates persuaded him to reluctantly accept it.

As a research supervisor, Bob had a zest for new projects and the ability to secure support and external collaborators for projects. He was an active member of AXAA, the Australian X-Ray Analytical Assn, editor of the AXAA journal (1982-1985) and National President (1996-1998). He was active at international conferences and his Research Workshops at the Denver, Colorado, X-Ray Analysis Conferences, were highly acclaimed. He published papers on x-ray powder diffraction, x-ray instrumentation, analytic techniques, neutron diffraction, radioactive waste disposal, electrical and magnetic properties of materials and the analysis of defects, strain and phase transitions in materials.

Bob was a Visiting Fellow at universities in England, the Inst. Laue-Langevin, the European Synchrotron Research Facility, Grenoble, France, the Nat'l Inst. of Standards & Technology, Gaithersburg, USA, and the Daresbury Synchrotron Lab, UK, where he introduced his Ph.D. students to the joy of long hours of measurement at great facilities.

Chris Kelaart