

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



W.L. Duax

At the opening ceremony of the IUCr Congress in Florence on August 23rd Philip Coppens will be awarded the Ewald Prize and will present a lecture. The award ceremony will be followed by a reception. Philip is an especially deserving recipient in that he, like Ewald, has not only conducted crystallographic research of the highest caliber, but has served the international community in many capacities, including President of the ACA (1978) and the IUCr (1993-1996). Philip embodies the spirit of the IUCr in that he has traveled to dozens of countries to describe his pioneering studies on high resolution electron density determination and *in situ* solid state reactions and has welcomed post doctoral trainees and collaborators from all over the world to work in his Buffalo laboratory.

With 2200 submitted abstracts and as many advance registrations, the Florence IUCr Congress promises to be the largest and most successful ever. Additional details appear on Page 30 and are on the XX Congress website (www.iucr2005.it/).

At the annual meeting of the Finance Committee, a very informative report was presented by Managing Editor, Peter Strickland, including information on the number of manuscripts submitted to the IUCr journals in 2004 from seventy-four countries, the acceptance rate of all co-editors and the total income and expenses for each journal. There has been an explosion in papers published in *Acta E*, the Unions first electronic journal. The content of *Acta E* grew by 22% (537 more papers in 2004 over 2003). Crystallographers in China were responsible for a phenomenal 39% of papers in *Acta E* in 2004. The list of ten countries with the highest number of papers published in *Acta E* includes two countries that are not yet members of the Union, Turkey and Malaysia. The rapid spread of crystallography in emerging countries is also reflected in the fact that Brazil ranks among the top 10 countries submitting papers to *Acta D* in 2004.

Articles published in IUCr journals in 2004 indicate that there are crystallographers working in 67 countries. Since we have only 40 member countries, we need to explore mechanisms to bring the other 27 countries into the Union. This could be a reason to explore the potential merit of expanding the size of the Executive Committee and to put in place procedures that would insure a balanced representation from the geographic areas of the Regional Affiliates, ACA, ECA, and AsCA.

The ACA reports that Argentina and Brazil have become its first country members. The guidelines for country membership include representation on the ACA Council, partial support for meeting attendees, complimentary student memberships in the ACA, and complimentary subscription to the IUCr journals. The benefits of membership (described in greater detail on the ACA website, www.hwi.buffalo.edu/ACA) will be rotated among laboratories within the member countries. Although the ECA has had member countries since its inception, this is a new program for the ACA.

A number of questions important to the IUCr will be under discussion at the Congress and General Assembly. At the Finance Committee meeting, John Helliwell, Editor in Chief, drew attention to two important issues, the need for a more effective policy for handling submitted manuscripts concerning crystallographic education and the challenge presented by the rapid growth of submissions to IUCr journals of manuscripts that are technologically sound but poorly written because the authors lack experience writing in English.

When the Executive Committee deliberated over the many nominations for membership of the next Executive Committee submitted by national committees, they decided to have only one nominee for each of the offices of the IUCr (President, Vice President, Secretary, Treasurer). Before 1990 there was only one candidate offered for any open position on the Executive Committee. In 1990, for the first time in IUCr history, the delegates to the Congress exercised their right to nominate additional candidates from the floor and elected two people who had not been endorsed by the Executive Committee, including the second woman ever to be elected to the Executive Committee. After that experience, the Executive Committee decided to nominate more candidates than the number of open positions in order to give the delegates to the Congress a choice. Some national crystallographic associations always provide more than one candidate for any open position. At the Florence Congress we should have an open discussion about whether there should be more than one candidate for each principal office in the IUCr in future elections.

The IUCr Newsletter is presently distributed to 17,000 crystallographers around the world. It would appear that there are twice that many scientists who are crystallographers, collaborators of crystallographers, co-authors of crystallographic papers, or have a genuine interest in our field. We would like to expand distribution of the Newsletter to include all these people. However we can't afford to double the cost of producing and posting hard copies. For this reason, we are experimenting with electronic distribution of the Newsletter. Electronic distribution expedites much more timely distribution of the information in the Newsletter. This issue of the Newsletter was placed on the IUCr Newsletter website (www.hwi.buffalo.edu/IUCr/IUCr-News/Home.html) two days after it was sent to the printer (approximately 5/3/05). Depending upon where you live, you will receive the hard copy version anywhere from three weeks to six months after that date. Printed copies will continue to be distributed to libraries, at national and international meetings, and will be sent to science funding administrators and individuals who wish to receive hard copies. We invite you to help expand our list of libraries and national meetings having crystallographic content.

Bill Duax, duax@hwi.buffalo.edu

LETTER TO THE EDITOR

Letter to the Editor

Dear Judy

Would the following be of interest? (During 1966-9 I was chairman of the original British 'X-ray Analysis Group'- so named by Bragg.)

I was interested to read the letter from Reuben Rudman about Prof. Belov and his poster at the 8th IUCr Congress. It reminded me of when Belov was over here in England in August 1960 for the 5th Congress, held in Cambridge. He was Vice-President at the time. One evening he asked me if he could get a newspaper. So I drove him round Cambridge until we found a news agent that was still open, and all was well. He told me that he wanted to try the crossword during the lectures when they were boring!

At that time visits from such people were not as easy-going as fortunately they now are, and I did wonder in retrospect what the newspapers would have made of it if an eminent Soviet academician had been found in a car crash late one night in Cambridge!

Edward Steward

Dear Edward,

I think that all such remembrances are of interest - they certainly are to me.

Judy

LETTER TO THE EDITOR

Letter to the Editor

Dear Judy,

It was a pleasure for me to receive and read No. 4 of Newsletters with the second part of "Crystallography in Russia". I have only one question: I failed to find a contribution from N. Andrushevsky among other papers. It was sent to you together with all others. Was it withdrawn or is to be printed separately in some next issue?

Leonid Aslanov

Dear Leonid,

Unfortunately, the contribution from N. Andrushevsky got misplaced somehow. We have found it and it appears on Page 24.

Judy

AWARDS AND PRIZES

Ewald Prize



Philip Coppens

The IUCr is pleased to announce that Philip Coppens (Dept. of Chemistry, State U. of New York at Buffalo, USA) has been awarded the seventh Ewald Prize for his contributions to developing the fields of electron density determination and the crystallography of molecular excited states, and for his contributions to the education and inspiration of young crystallographers as an enthusiastic teacher by participating in and organizing many courses and workshops.

The presentation of the Ewald Prize will be made during the Florence Congress Opening Ceremony on August 23, 2005.

AWARDS AND PRIZES

Wlodawer receives doctor honoris causa



Alexander Wlodawer

It is a pleasure to communicate to the crystallographic community that with the approval of the Academic Senate, the Technical U. of Lodz has awarded Alexander Wlodawer the privileges and title of Doctor Honoris Causa. The presentation ceremony took place October 1, 2004, as part of the inauguration of the academic year 2004/2005. This honor is bestowed on only the most distinguished scientists, with the previous recipients in the field of crystallography being Herbert Hauptman and William Duax.

Alex was one of the pioneers of the applications of synchrotron radiation and neutron diffraction in protein crystallography. His name is permanently associated with the exciting history of the discoveries of the secrets of the molecules of life with the use of the research arsenal of crystallography. Born and educated in Poland, Alex obtained his Ph.D. with David Eisenberg at UCLA. Since 1987 he has been the Head of the Macromolecular Crystallography Lab at the National Cancer Inst. (NCI), Frederick, MD, USA. His research at the NCI is marked with several discoveries in structural biology, with consequences in pharmacology and medicine. The most notable is the determination in his laboratory of the structure of two retroviral enzymes, including the structure of retroviral protease, which provided the foundation for the spectacular success in the rational design of drugs for the treatment of AIDS.

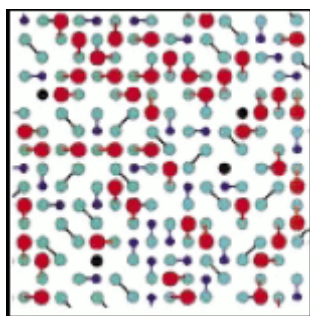
To commemorate the award, Grzegorz Bujacz organized a scientific symposium on “Crystallography of Biomolecules”, with participation of all leading Polish protein crystallographers. The symposium took place at the Institute of Technical Biochemistry, Faculty of Biotechnology and Food Sciences of the Technical U. of Lodz.

Grzegorz Bujacz (Lodz, Poland)

Structures, phase transitions and orientational properties of the C₆₀ monomer and polymers

Structures, phase transitions and orientational properties of the C₆₀ monomer and polymers

Acta Cryst. (2005). A61, 62-76



Model distribution of C₆₀ dimers: a precursor stage of the high-pressure high-temperature polymerization (C₆₀ are represented as circles).

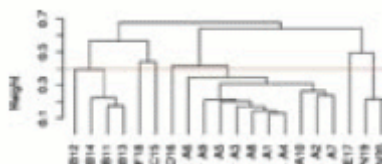
The high symmetry and round shape of the fullerene molecules induce orientational phenomena that play an important role in the properties of the fullerene compounds. This is illustrated in this review, which is focused on the orientational properties of C₆₀ monomer and polymer structures. The peculiar pressure-temperature orientational phase diagram of pristine C₆₀ is first described. Then, the polymerization processes and the various structures obtained under high-pressure high-temperature conditions or via doping by alkali metals are summarized.

Roger Moret

IUCR JOURNALS NEWS

Method for the computational comparison of crystal structures

***Acta Cryst.* (2005). B61, 29–36**



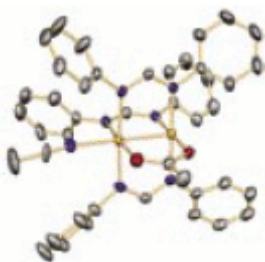
Dendrogram for the test data set, showing perfect agreement with known structure classification. A new method for assessing the similarity of crystal structures is described. A similarity measure is important in classification and clustering problems, in which the crystal structures are the source of information. Classification is particularly important for the understanding of properties of crystals, while clustering can be used as a data reduction step in polymorph prediction. The method uses a radial distribution function that combines atomic coordinates with partial atomic charges.

E. L. Willighagen, R. Wehrens, P. Verwer, R. de Gelder and L. M. C. Buydens

A paramagnetic precursor for polymeric supramolecular assemblies based on multiply bonded dimetal units: μ -acetato-acetonitriletris(μ -N,N'-diphenylformamidinato)diruthenium tetrafluoroborate dichloromethane hemisolvate

A paramagnetic precursor for polymeric supramolecular assemblies based on multiply bonded dimetal units: μ -acetato-acetonitriletris(μ -N,N'-diphenylformamidinato)diruthenium tetrafluoroborate dichloromethane hemisolvate

Acta Cryst. (2005). C61, m71-m73



The cation of a paddlewheel species with an Ru_2^{5+} core and a labile equatorial acetate ligand. An acetonitrile molecule occupies an axial position.

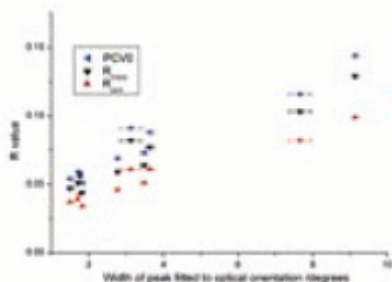
Metal-metal bonded compounds having an Ru_2^{5+} core and a paddlewheel structure can have a variety of electronic configurations because the δ^* and π^* orbitals are close in energy. Configurations such as $Q\delta^{*2}\pi^*$, $Q\delta^*\pi^{*2}$ and $Q\pi^{*3}$ ($Q = \sigma 2\pi^* 4\delta^{*2}$) are possible and each is expected to possess a unique Ru—Ru distance and different magnetic properties. Such properties can be incorporated into supramolecular arrays by joining diruthenium units with appropriate linkers in reactions using corner piece precursors having mixed sets of labile and non-labile ligands. For example, a precursor with two cis non-labile ligands can form squares and one such as the title molecule, which has three non-labile formamidinate ligands and a labile acetate group, can form “dimers of dimers”.

P. Angaridis, F. A. Cotton, C. A. Murillo and X.-P. Wang

IUCR JOURNALS NEWS

A new method for predetermining the diffraction quality of protein crystals: using SOAP as a selection tool

Acta Cryst. (2005). D61, 130-140

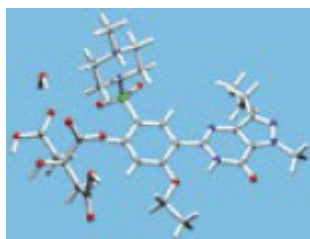


A polarising light microscope (the Metripol) is used to quantitatively assess the optical quality of crystals of three different proteins (HEWL, glucose isomerase and the 2F1-3F1 module pair of human fibronectin). By comparing variations in the slow optical axis position (SOAP) with indicators of diffraction quality [$\sigma(I)$, R_{meas}], it is shown that the optical properties of a protein crystal can provide a non-invasive method of predetermining likely crystal diffraction quality before X-ray data collection is undertaken.

R. L. Owen and E. Garman

Sildenafil citrate monohydrate

***Acta Cryst.* (2005). E61, o489–o491**



The name of the anti-impotence drug Viagra is well known to many people, even to those who have nothing to do with chemistry or pharmacology. A number of investigations on this compound, with the pharmaceutical name sildenafil citrate, have already been published. As the knowledge of the molecular conformation is essential for understanding structure–activity relationships, it is surprising that its crystal structure has not been previously reported. This paper closes this gap by reporting the crystal structure of the monohydrate.

H. S. Yathirajan, B. Nagaraj, P. Nagaraja and M. Bolte

IUCR JOURNALS NEWS

Expression, purification and X-ray crystallographic analysis of thioredoxin from *Streptomyces coelicolor*

***Acta Cryst.* (2005). F61, 164-168**



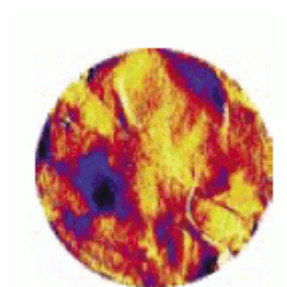
Overall structure of the TrxA molecule from *S. coelicolor*. α -Helices are shown in purple and β -strands in yellow.

The Gram-positive bacterium *Streptomyces coelicolor* contains three thioredoxins that are involved in unknown biological processes. *trxA* from *S. coelicolor* was cloned and expressed in *Escherichia coli* and the protein purified and crystallized using the hanging-drop method of vapour diffusion. The crystal structure of thioredoxin A has been determined at 1.5 Å resolution using synchrotron radiation. The crystal exhibits the symmetry of space group $P2_12_12$, with unit-cell parameters $a = 43.6$, $b = 71.8$ and $c = 33.2$ Å.

Petra Stefankova, Jana Maderova, Imrich Barak, Marta Kollarova and Zbyszek Otwinowski

Distribution and Burgers vectors of dislocations in semiconductor wafers investigated by rocking-curve imaging

J. Appl. Cryst. (2005). **38**, 91-96



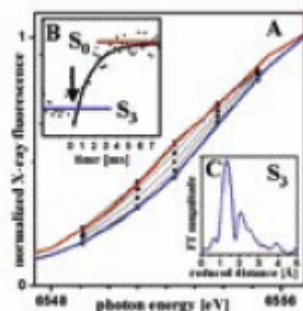
A map of local lattice curvatures, measured by parallel X-ray microdiffraction imaging on a 2-inch GaAs wafer.

This article presents a method of quantitatively visualizing dislocation distributions in semiconductor wafers by parallel X-ray microdiffraction imaging. Unlike previous techniques, the method is both non-destructive and model-free and measures a vectorial Burgers vector density rather than scalar dislocation density. Data analysis is based on local changes in Bragg peak positions as a typical signature of dislocations. Results obtained from InP and GaAs wafers on beamline ID19 at the ESRF demonstrate the potential of the technique. The effective spatial resolution, set to 80 μm for initial experiments, can be significantly enhanced in the future.

Daniel Lübbert, Claudio Ferrari, Petr Mikulík, Petra Pernot, Lukas Helfen, Nicola Verdi, Dušan Korytár and Tilo Baumbach

A novel BioXAS technique with sub-millisecond time resolution to track oxidation state and structural changes at biological metal centers

J. Synchrotron Rad. (2005). **12**, 35-44



Time-resolved BioXAS on the Mn-complex of photosynthesis at 18°C. (A) Mn XANES spectra spaced by 500 μ s (symbols) during the S₃→S₀ transition. (B) X-ray transient at 6553 eV at 200 μ s resolution (arrow, laser flash). (C) Fourier-transformed S₃-state EXAFS measured within 200 ms after the laser flash. X-ray absorption spectroscopy (XAS) to study metal cofactors in enzymes is an increasingly important tool in structural biology. Frequently, characterization of short-lived reaction intermediates is a decisive step in unraveling the catalytic mechanism. A novel approach for time-resolved BioXAS to trace intermediates is described. For the first time, XANES and EXAFS spectra were obtained, for the tetra-manganese complex of oxygenic photosynthesis, within micro- to milliseconds after population of semi-stable states by laser-flash excitation at room temperature. Now the road is open for “real-time” BioXAS investigations.

M. Haumann, C. Müller, P. Liebisch, T. Neisius and H. Dau

MEETING REPORT

ECM22

Budapest, Hungary, August 2004



The 22nd European Crystallographic Meeting took place in the Convention Centre of the Eötvös Loránd U., Budapest, Hungary, August 26-31, 2004 exactly thirty years after the 2nd European Crystallographic Meeting was organized in Keszthely, Hungary.



Sydney Hall, Editor of International Tables for Crystallography Vol. G and Yuji Ohashi, President of AsCA. Scientific organization and coordination of the conference were performed by the Single Crystal X-ray Diffraction Group of the Inst. of Structural Chemistry, Hungarian Academy of Sciences under the auspices of the European Crystallographic Assn and the IUCr. In the absence of a Hungarian Crystallographic Assn, the Hungarian Chemical Society (A. Kálmán, President) and Chemol Travel provided professional help. The Organizing Committee consisted of the members of the Hungarian Nat'l Committee of IUCr; the ECA President, H. Fuess, Vice- and Past-presidents, M. Jaskolski and C. Lecomte; representatives of previous ECM's, K. Lewinski and A. Roodt. Both the Organizing and Program Committee were chaired by A. Kálmán. The Program Committee consisted of H. Fuess and G. Heger; along with three representatives who were responsible for chemistry (A. Kálmán), physics (G. Faigel) and biology (V. Fülöp). The representatives of the thirteen Special Interest Groups (SIG) of ECA (H. Graafsma, V. Petrícek, U. Kolb, H.S. Effenberger, J.R. Helliwell, R. Boese, E. Mittemeijer, A.L. Spek, M.V. Kovalchuk, A. Polian, P.A. Thomas, and F.J. Lahoz) were also on the Program Committee.



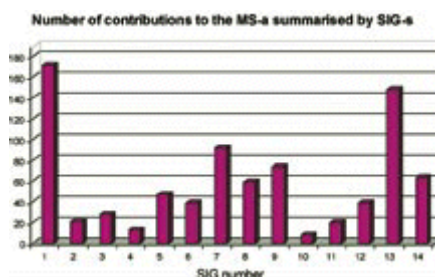
George Sheldrick (right) received the MaxPerutz award of ECA in 2004 for his seminal contributions to the development of direct methods and for transfer of the methodology into a straightforward procedure for solving small molecule structures, as well as for his work in biological crystallography, in the areas of structure solution based on anomalous phasing and in the refinement of protein structures at atomic resolution.

At the Opening Ceremony Hartmut Fuess, Sándor Görög (President of the Dept of Chemistry of the Hungarian Academy of Sciences) and Bill Duax (President of the IUCr) greeted the participants. The "Max Perutz Prize" was awarded to George Sheldrick who gave a short talk since he was also a keynote speaker. At the Opening Ceremony the Rajkó Ensemble played music pieces from Franz Liszt and Johannes Brahms.



Hans-Beat Bürgi and Dieter Schwarzenbach in discussion during the coffee break.

The scientific program ran for four days. The morning and evening keynote sessions consisted of 16 lectures by eminent scientists based on the proposals of the SIGs: Macromolecular Crystallography (G.M. Sheldrick, W.D. Schubert, and D. Stuart); Molecular Interaction and Recognition (J.L. Atwood, G. Klebe), Crystallography under Extreme Conditions (S. Klotz, M.I. McMahon; Molecular Structure and Chemical Properties (J. Elguero, J.A.K. Howard); Charge, Spin & Momentum Density (U. Pietsch), Aperiodic Crystals (S. van Smaalen), Electron Crystallography (A.S. Avilov), Instrumentation and Experimental Techniques (C. Nave), Powder Diffraction (C. Riekel), Crystallographic Computing (R.J. Read) and Material Science (J. Evans).



Each microsymposium lasted two hours. Most of the chairs and co-chairs followed the suggestion of ECA to have two thirty minute comprehensive lectures followed by three twenty minute oral research reports. This allowed participants the opportunity to change microsymposia between talks. Five parallel sessions, forty microsymposia, with all together 203 lectures, presented high quality science. The number of contributions received for each microsymposia is shown in Fig. 1.



On board the "Europe" at the ECM22 conference dinner: Anders Liljas, his wife, Hank Schenk, Andrea Sharpe, Davide Viterbo, Giuseppe Filippini, and Maria Teresa Duarte.

Over 400 posters were presented in two poster sessions. Both poster sessions lasted two days with two hours for discussion in the afternoons. Four different poster prizes were awarded. RCSB PDB: For the best graduate / undergraduate student poster presentation involving macromolecular crystallography (Jacques-Philippe Colletier), CCDC: Three prizes in chemical crystallography (Ayesha Jacobs, Thammarat Aree, Zoran Stefanic), Oxford Cryosystem: Low Temperature Prize for describing applications involving low temperature crystallography (Philippe Fernandes), and Sigma-Aldrich (Fluka Chemistry): Youth Excellence Award to a young participant (Oleg Kovalev).



Howard Flack and Michael Hursthouse were talking about pre-print, e-print and institutional servers. Flack is the chair of the IUCr's Committee on Electronic Publishing, archiving and dissemination of information, while Hursthouse has an interesting project running for the depositing, preservation and archiving of crystal structures.

The Abstract Book is available in different forms. A printed and CD version were distributed to participants at the venue as supplementary material of *Acta Cryst. A*, **60**, Part a1, pp. s1-s308, 2004, and, for the first time in the history of ECM Meetings, they are available on the conference website (www.ecm22.mtesz.hu/).



Closing ceremony. The Organizers from left to right: Alajos Kálmán, Franciska Morlin, Beáta Androsits, Nikoletta Báthori, László Fábián, Petra Bombicz.

The organization of ECM22 was fully electronic. Registration was highly encouraged to be performed via the conference website. Abstract submission was only possible using the on-line abstract submission system. The International Bursary Committee performed its task using a specially designed website allowing members to work together sitting in their own country. An internet corner with 22 computers and a slide check room were also available during the meeting. Wireless internet access was provided to the participants in the main hall. Both the first and second circulars advertising the meeting were published in the *IUCr Newsletter*.



Handing over the relay: Prof. Alajos Kálmán (chair of ECM22) and Prof. Luc Van Meervelt (chair of ECM23). A three-day satellite conference, "Crystallography at the Start of the 21st Century: Mathematical and Symmetry Aspects", preceded ECM22 at the same venue: it was organized by Massimo Nespolo (U. Henri Poincaré, Nancy, France).

The IUCr Executive Committee Meeting took place August 24-26 in Budapest before the European meeting. ECM22 hosted several events during the conference: the ECA Executive Committee, the IUCr Journals Commission, the Oldenbourg Verlag, the Daresbury synchrotron radiation meeting for potential users, and all 13 Special Interest Groups of ECA.

A four and a half day exhibition accompanied the conference. Thirty companies offered products, equipments, books, and databases. The location of the exhibition area was centrally located on the way

to the lecture theatres; coffee, tea and cakes were served on this area. Posters were displayed in the gallery of this spacious hall illuminated by natural light through the glass roof.

Thanks to the generosity of IUCr and ECA over seventy students and young researchers were partially supported to attend the meeting. A student mixer was also organized to foster new contacts and friendships with possible scientific fruits in the future. A concert entertained the participants in St. Matthias Church one evening. The piece, the Hungarian Coronation Mass, was composed by Franz Liszt for the coronation of the Emperor of Austria and the Empress Elisabeth as King and Queen of Hungary that premiered in this church on June 8, 1867. The closing ceremony and conference dinner took place on board the boat "Europe" cruising on the Danube, providing a panoramic view of the capital. An optional Hungarian dinner, accompanying persons' tour every day and organized programs on the excursion day completed the social programs.

Although countries of Africa and the Middle-East belong to the ECA, scientists from 45 countries of five continents attended ECM22. The highest number of participants arrived from the UK, Germany, France, Switzerland and the USA. Nearly five hundred researchers, 150 students, exhibitors and some 60 registered accompanying persons contributed to the success of the 22nd European Crystallographic Meeting. The efforts and hard work of the members of the Program and Organizing Committee, the official organizers and the contributions of the sponsors are highly appreciated.

For more information, visit www.ecm22.mtesz.hu.

Petra Bombicz, ECM22 Secretary and Alajos Kálmán, ECM22 Chair

MEETING REPORT

International crystal growth

Berlin, Germany, August 2004



The Twelfth Int'l Summer School on Crystal Growth (ISSCG-12)" was held August 9 -13 at the Seminar and Meeting Centre Akademie Berlin-Schmoeckwitz in Berlin, Germany. The school was held in conjunction with the 14th Int'l Conference on Crystal Growth (ICCG-14) held in Grenoble, France. Chairmen of the school were G. Müller (U. Erlangen-Nürnberg, Germany), J.-J. Metois (U. Marseille, France), and P. Rudolph (IKZ Berlin, Germany).



Participants at the Twelfth International Summer School on Crystal Growth (ISSCG-12).

The meeting was jointly organized by the Deutsche Gesellschaft für Kristallzuechtung und Kristallwachstum (DGKK) and Groupe Francais de Croissance Cristalline (GFCC) under the auspices of the Int'l Organization of Crystal Growth (IOCG). The Inst. for Crystal Growth in Berlin (IKZ) was responsible for local organization. There were 66 students from 20 countries in Europe, Asia and South America supported by grants. This represents about 50 % of all participating students. 3 participants received full coverage of all expenses (including travel fees) from the InWent GmbH. All students that received grants presented posters.

The lectures have been published by Elsevier Science B.V. "Crystal Growth - from Fundamentals to Technology" edited by G. Mueller, J.J. Metois and P. Rudolph, July 2004, 422 pages, ISBN 0-444-51386-8. Each participant received a copy. ISSCG-12 covered tutorials and scientific topics in crystal growth and materials science. 169 scientists from 28 countries of four continents participated.

Both the technical program, with more than 30 lectures and tutorial seminars, and the support for students would not have been possible without generous contributions from: DGKK, European Space Agency (ESA), IKZ, IUCr Commission on Crystal Growth and Characterization of Materials, ICCG-14, Deutsche Forschungsgemeinschaft (DFG), Deutsche Gesellschaft fuer Kristallographie (DGK), FhG IISB Erlangen Crystal Growth Lab, WISTA Management GmbH Berlin-Adlershof, Internationale Weiterbildung und Entwicklung GmbH (InWent).

ISSCG-12 was organized to encourage research in the field of crystal growth. Information about this meeting was distributed by the German press information service (IDW) before the meeting. During the school a press conference was held and several newspapers published articles about the school. The interest of politicians was expressed in a welcome speech by the lord mayor of Köpenick, the district of Berlin where ISSCG-12 was located.

The conference made an important contribution to the further development of friendly relations among the community of nations.

Georg Müller, Jean-Jacques Metois, and Peter Rudolph

MEETING REPORT

EPDIC IX

Prague, Czech Rep., August 2004



The 9th European Powder Diffraction Conference and the Size-Strain IV workshop were held together in Prague at the Czech Technical U., Faculty of Civil Engineering.

The workshop, held August 31 - September 2, followed the tradition of previous conferences in Slovakia (1995), Germany (1998) and Italy (2001). The workshop was organized around X-ray powder diffraction, line-profile analysis and determination of grain size and strain including its relation to texture and stress. Main lectures given by R. Kuzel, N. Armstrong and P. Scardi were devoted to reviews of dislocation and size diffraction line broadening as well as whole powder pattern modeling for the study of nanocrystalline and imperfect materials. Approximately 90 participants attended the workshop. The XRD analysis of nanocrystalline powders and thin films as well as severely deformed materials was discussed (D. Rafaja, R. Pielaszek, Z. Kaszukur, J. Gubicza, A. Leineweber, J. Rodriguez-Carvajal, A. Borbély, A. Boulle). The workshop ended with a discussion, organized by the workshop chair, P. Scardi, on the problems of line profile analysis. Participants felt that the tradition of working Size-Strain meetings should definitely continue.



EPDIC IX started with a workshop organized by L.M. Cranswick. He is famous for his enthusiasm in the field of (mainly free) crystallographic software distribution, maintaining the CCP14 site as the CCP14 secretary for many years and for organizing software workshops during the IUCr and ECA meetings. After several workshops on structure refinement, this time the program was split into two half-day sessions – size-strain software and phase analysis software. The workshop was free for the Size-Strain and EPDIC registered participants and more than 150 participants listened to 14 short presentations. Both commercial (Bruker Topas, Panalytical HighScore, Bergmann BGMN) and free software were presented. Some of it is of general purpose including size-strain and phase analysis, other is rather special. Both phenomenological size-strain and phase analysis is included in Rietveld type programs such as Fullprof (Rodriguez-Carvajal) and Maud (Lutteroti). It also seemed appropriate to discuss line profile analysis and whole powder pattern modeling (fitting) including a physically realistic microscopic description. This approach was presented by M. Leoni (PM2k) and G. Ribárik (CMWP - fit).

The third workshop on new trends in the development of databases was organized by J. Faber (ICDD).



No one went hungry at the socials.

The program started each day with two plenary lectures. In total, there was six invited talks: A. Fitch (ESRF, Grenoble) on high-resolution diffraction, U. Welzel (Stuttgart) on diffraction stress analysis, L. McCusker (Zurich) on exploiting preferred orientation to resolve overlapping reflections, T. Ungar (Budapest) on nanocrystalline materials, G. Vaughan (ESRF) on a multicrystal approach to crystal structure solution and H. Ehrenberg (Darmstadt) on *in-situ* characterization of materials.



Vincent Favre-Nicolin

The plenaries were followed by two parallel sessions. All posters were displayed during the entire conference. Poster sessions during and after lunch, gave enough time for discussion. The topics of the parallel microsymposia were: structure solution from powder diffraction; methods and application, stress, strain and texture analysis, neutron diffraction - instruments and applications, phase transitions, non-ambient conditions, phase analysis, structure and properties of bio-materials, nanocrystalline materials, metals and alloys, minerals, thin films, techniques and instruments, indexing powder patterns and software.



Commercial exhibitions were open during most of the conference. Two sponsors, Panalytical and Bruker enabled the organizers to offer financial assistance to quite a few participants. Participation of young scientists was supported by the IUCr. Strong support was also given by the ICDD and Unisantis. The organizers would like to thank all of the sponsors, Huber, GBC, Stoe, XOS, GE Inspection Technologies, Inel, Osmic, Zentiva, Anton Paar, Oxford Cryosystems and Röntgenlabor Dr. Ermrich.



Radomir Kuzel

During the conference two meetings were held: CPD (Commission for Powder Diffraction of the IUCr) and EPDIC committee (identical with a SIG8 of the ECA). In the latter meeting a new chairman of the committee was elected, J. Rius (Barcelona, Spain) as well as two vice-chairs - P. Scardi (Trento, Italy) and R. Cernik (Manchester, UK). P. Scardi is also the committee secretary.

The conference opened with a welcome evening in the Prague Congress Center and the traditional EPDIC award lecture. The award, sponsored by Panalytical, was given to Vincent Favre-Nicolin, the author of the FOX program and Crystal Object system. The lecture was followed by a musical performance by the Z-band, a mixed voice choir of the Prague secondary school.

The last day included a train trip to Pilsen and a tour and dinner in the Pilsen brewery.

It is difficult to select a time for the conference that doesn't conflict with IUCr and ECA meetings. It was decided to attach it to the Budapest ECM meeting, which was convenient for some participants and companies but not for others. In the opinion of the EPDIC IX organizers it would be very reasonable, if the ECA would meet in the year following the IUCr Congress and in the following year EPDIC and other specialized conferences and meetings could be organized. Future EPDIC organizers should try to attract more people from industry because this was the original idea behind the conference. At any rate,

participation of more than 320 people from 36 countries in Europe, North and South America, Africa, Asia and Australia was quite good. In addition to 54 local participants, the highest number came from Germany (49), France (19), Sweden (18), UK (16), Hungary, Austria, and the Netherlands (13), Italy and USA (12) and Poland (10).

Additional information, including conference abstracts in html format, photos and a few video clips, is available at www.xray.cz/epdic. Approximately one hundred papers, 6 pages each, have been submitted for publication in the conference proceedings. They should appear within one year in a special issue of *Zeitschrift für Kristallographie*.

I would like to acknowledge the excellent work of the organizing committee. Namely, secretaries P. Rezacová and I. K. Smatanová, treasurer: J. Hašek, secretary for commercial presentations: Z. Šourek, and to members of the committee responsible for: accommodations - I. Císarová, refreshments: R. Králová, A. Župranová, trips: D. Havlíček, poster sessions: N. Ganey, also to S. Daniš, R. Gyepes, R. Novák, L. Kopecký.

The next conference, EPDIC X, will be held in September 2006 in Geneva, Switzerland. Information is available by contacting the organizer, R. Cerny, Radovan.Cerny@cryst.unige.ch.

R. Kuzel, Chairman of EPDIC IX

MEETING REPORT

XTOP 2004**Pruhonice, Czech Republic, September, 2004**

The 7th Biennial Conference on High Resolution X-Ray Diffraction and Imaging – XTOP 2004 was held September 7–10, in the Congress Centre Floret in the Prague suburb of Pruhonice. Previous conferences were held in Switzerland (1990), Germany (1994), Italy (1996), Durham (1998), Poland (2000), and France (2002).



The conference covered a wide range of topics including theory of X-ray scattering, high-resolution X-ray diffraction, X-ray reflection, grazing-incidence scattering, X-ray scattering from thin films and nanostructures, X-ray topography, X-ray phase contrast imaging and other X-ray imaging techniques and instrumentation for all these methods. The Czech and Slovak Crystallographic Assn organized the meeting in cooperation with the Inst. of Physics, Academy of Sciences of the Czech Republic, Prague, Masaryk U., Brno and Charles U., Prague.



Andrew Lang

XTOP 2004 featured pre-conference tutorial lectures presented by experts in the field: “Imaging with hard synchrotron radiation” (J. Härtwig, Grenoble), “High-resolution X-ray diffractometry: Determination of strain and composition” (J. Stangl, Linz), “X-ray grazing-incidence scattering from surfaces and nanostructures” (U. Pietsch, Potsdam) and “Hard X-ray optics” (J. Hrdy, Prague).

The scientific program was divided into 11 oral and 2 poster sessions. There were nine 45-minute invited talks, thirty-four 20-minute orals and 104 posters (displayed for the whole meeting).

The invited lectures included: “Coherent diffraction analysis of dislocation arrays in *geSi* thin films” (I. Robinson, Urbana), “X-ray scattering of nanostructured soft matter films” (W. de Jeu, Amsterdam), “Some trends of hard x-ray synchrotron radiation imaging” (J. Baruchel, ESRF), “Overgrowth phenomena studied by anomalous scattering combined with high-resolution reciprocal space mapping” (T. Schülli, Grenoble), “*In situ* x-ray studies of the morphology, organization and internal structure of growing nanoparticles” (G. Renaud, Grenoble), “Femtosecond X-ray diffraction” (J. Wark, Oxford), “Magnetic transmission soft X-ray microscopy: looking into nanomagnetism at short length and fast time scales” (P. Fischer, Stuttgart), “X-ray waveguides as nano-focusing devices” (W. Jark, Trieste), and “X-ray standing wave imaging” (J. Zegenhagen, Grenoble). Poster topics generated a lot of interest and discussion could be heard not only during sessions but over an evening glass of beer. The full list of all contributions together with their abstracts are available at the conference website www.xray.cz/xtop.

During the meeting, A. Lang, honorary guest of XTOP 2004, one of the pioneers of X-ray topography who gave his name to the popular topographic technique, celebrated his 80th birthday. A. Authier reviewed Prof. Lang's career and his invaluable contribution to the development of the field.

A special issue of *Journal of Physics D: Applied Physics* containing full peer reviewed high-level original contributions from XTOP will appear in 2005.

In total, 147 official delegates from 16 countries attended the conference. Of these, 13 students and young scientists from Europe and Latin America received sponsorship from the IUCr. Others were partially or totally supported thanks to other sponsors. The commercial exhibition included booths of all of the sponsors.

The general scientific and presentation standards of contributions was high. The efforts of all members of the local organizing committee were also a big factor in the success of this event.

XTOP 2004 ended with a conference dinner in the Prague Congress Centre with a splendid view of Prague Castle at sunset. Prof. Baumbach and his group from the Inst. for Synchrotron Radiation at the Forschungszentrum Karlsruhe will organize the next conference, XTOP 2006, in Germany.

Zbyněk Šourek and Václav Holý

MEETING REPORT

6th Singapore national crystal growing challenge

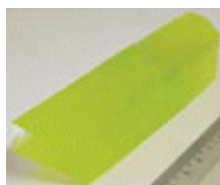
6th Singapore national crystal growing challenge

Singapore, September, 2004



$\text{K}_3[\text{Fe}(\text{CN})_6]$ bar (weight, 217.77 g and measuring $17.5 \times 2.7 \times 3.1 \text{ cm}^3$)

The wonderful colors, well-developed faces, sharp edges and artistic forms displayed by crystals of naturally occurring minerals have given rise to their use in precious jewelry and admiration as art objects. Growing crystals of a desired size and shape is considered an art as well as a science. The Dept. of Chemistry at the National U. of Singapore and Singapore National Inst. of Chemistry (SNIC) have organized the 6th Singapore National Crystal Growing Challenge for secondary school, junior college and polytechnic students. The students had an opportunity to show their creativity in the form of crystals and learn the science of growing crystals. Further, growing your own crystals can be a creative way to learn many aspects of basic physics, chemistry, geology and biology. Above all crystal growing is lots of fun!



KH_2PO_4 crystal (weight, 201.28 g and dimensions, $14.1 \times 2.8 \times 2.9 \text{ cm}^3$)

There were three categories in this year's competition, Junior (for secondary school students), Senior (for Junior college and polytechnic students) and Open levels. For the junior level category, the students were asked to grow crystals of blue-green copper acetate monohydrate, $\text{Cu}(\text{CH}_3\text{CO}_2)_2 \cdot \text{H}_2\text{O}$. The senior level students were challenged to grow colourless sodium nitrate crystals. The students in these categories were frustrated by the fact that they were unable to grow very big crystals like alum in the previous contest. On the other hand, the students for the open level were given the task of growing the longest single crystal so to exercise their creativity and scientific knowledge. The ratio of the length to the average of the other two dimensions was used as an important factor for judging. The greenish-yellow potassium chromate doped KDP (KH_2PO_4) crystal (weight, 201.28 g and dimensions, $14.1 \times 2.8 \times 2.9 \text{ cm}^3$) was chosen as the open category champion due to its scientific ingenuity over the first runner-up, a dark blood-red crystal of $\text{K}_3[\text{Fe}(\text{CN})_6]$ weighing 217.77 g and measuring $17.5 \times 2.7 \times 3.1 \text{ cm}^3$. In Singapore, this crystal growing challenge has been a very popular event among secondary-schools. This year, there were 168 entries from 68 educational institutions. This year's competition was once again generously sponsored by Bruker Singapore Pte Ltd, Lee Foundation of Singapore and the Singapore National Academy of Science. Details of this challenge and the names of the winners are available at the website: www.chemistry.nus.edu.sg/ncgc/index.html.

Jagadese J. Vittal and Edward R.T. Tiekink

MEETING REPORT

Hellenic Crystallographic Association

Athens, Greece, October, 2004

The Hellenic Crystallographic Assn (HeCrA) organized two events in 2004. Its 2nd conference at NCSR “Demokritos” was held October 15-16, 2004. Oral and poster presentations covered many aspects of crystallography. Topics included supramolecular organization in archeological samples (G. Tsoucaris, Louvre, Paris), photonic crystals (N. Stefanou, U. of Athens), combining electron microscopy and X-Ray techniques (J. Navaza, CNRS, Paris), apolipoprotein peptide models (M. Sakarellos-Daitsiotis, U. of Ioannina), structural studies of nicotinic acetylcholine receptor (S. Tzartos, U. of Patras), structural investigations of titin (M. Wilmanns, EMBL, Hamburg), epigenetic DNA code (E. Moudrianakis, Johns Hopkins U., Baltimore), cyclodextrin structure (K. Yannakopoulou, NCSR Demokritos, Athens), powder diffraction of proteins (I. Margiolaki, ESRF, Grenoble), microporous coordination polymers (S. Skoulika, U. of Ioannina), thermostable proteins (C. Vorgias, U. of Athens), complexes of glucogene phosphorylase b (E. Chrissina, National. Res. Found., Athens), multi-dimensional approach to molecular replacement (N.M. Glykos, U. of Thrace, Alexandroupolis).

The conference was preceded by the 2nd Workshop of the HeCrA on the Rietveld Method, October 13-14, which took place at the Dept. of Physics of the U. of Athens and was organized by M. Calamiotou (Dept. of Physics), V. Perdikatsis (Dept. of Mineral Resources Engineering, Technical U. of Crete), A. Stergiou (Dept. of Physics, U. of Thessaliniki), and V. Psicharis (Inst. of Material Sciences, NCSR Demokritos). The workshop was attended by 22 graduate students and postdoctoral fellows.

The association acknowledges the financial assistance of the sponsors and the IUCr for their contribution to young scientists in order to attend the workshop and conference. The titles of all presentations of the conference, programs of the conference and workshop along with photographs from both events can be found at www.hecra.gr.

Irene Mavridis

President, Hellenic Crystallographic Assn

MEETING REPORT

BioCrys2004

Oeiras, Portugal, November 2004



The second BioCrys Course on 'Fundamentals of modern methods in biocrystallography', organized by M.A. Carrondo (ITQB Oeiras, Portugal) and T. Schneider (FIRC Inst. of Molecular Oncology, Milan, Italy) took place at the Inst. de Tecnologia Química e Biológica in Oeiras, Portugal from November 19-26, 2004. The course was supported by the MAXINF network (www.maxinf.org, HPRI-CT-2000-40021), the SPINE project (www.spineurope.org, QLG2-CT-2002-00988), and the IUCr. It brought together 34 students and 19 tutors from 16 different countries.

Subtitled 'What you always wanted to know about crystallography but never dared to ask ...', the course aimed at teaching fundamental theoretical concepts of macromolecular crystallography to scientists in the early stage of their crystallographic careers. This is particularly important due to the rapid development of the field and the fact that many young researchers do not receive a formal education in crystallography. Additionally, with the introduction of high-throughput methods, the need to understand and grasp the theory behind modern methods will be critical to tackle the difficult problems that will not be solved by automated procedures.

Lectures and tutorials covered topics from the cooling of crystals to the validation of the final structural model. Lectures were held in the morning and interactive practicals and tutorials in the afternoon. For the computational tutorials, 18 Linux-computers were set up by P. Matias and M.M. Rato (ITQB, Portugal). Tutors or invited speakers presented evening lectures about a current topic in structural biology.

E. Hough (U. Tromsø, Norway) laid out the basics of crystallography in real and reciprocal space. C. Hermes (EMBL Hamburg, Germany) gave an overview of the principles of X-ray sources and detectors and E. Garman (Oxford U., UK) lectured and demonstrated the practical side of crystal cooling and data collection. K. Cowtan (U. York, UK) guided the students through the world of structure factors and how they relate to electron densities in his web-based tutorial (www.yorvic.york.ac.uk/~cowtan/sfapplet/sfintro.html). Understanding the basics was complemented by a tour of crystallographic resources on the internet, presented by F. Enguita (ITQB Oeiras, P).

Strategic questions of data collection and the principles of data processing were addressed by Z. Dauter (Argonne Nat. Lab., USA) and A. Leslie (MRC Cambridge, UK). This included a tutorial on 'How to read (and understand...) the International Tables' given by Z. Dauter.

Lectures and tutorials focused next on experimental phasing. G. Leonard (ESRF Grenoble, France) gave an introduction to the use of anomalous scattering in macromolecular crystallography. The MIR-method was discussed and later demonstrated in a tutorial by C. Vornrhein (GlobalPhasing Cambridge, UK). The substructure solution process and MAD-phasing were covered by T. Schneider (IFOM Milano, Italy). K. Cowtan discussed the principles of different density modification techniques used for phase improvement, followed by Z. Dauter, who explained various aspects of SAD-phasing. Molecular Replacement was introduced and discussed with the help of examples by P. Matias. T. Schneider lectured on refinement and model precision and C. Frazão described how the particular problems encountered

with twinned crystals can be tackled. Tutorials on this day were still concerned with phasing (MAD phasing by T. Schneider and density modification by K. Cowtan).

The central topics of the last two days were molecular replacement and both manual and automated model building. A. McCoy (Cambridge U., UK) introduced the basic concepts of maximum likelihood as used in crystallography and then led the students through the practical use of these in molecular replacement. Automated model building and refinement was discussed both from a methodological and practical point of view by A. Perrakis (NKI Amsterdam, NL). M. Kjeldgaard taught the principles and practicalities of manual model building. The discussion of model building was complemented by overviews of what can be achieved with atomic resolution crystallography by K. Wilson (York Univ., UK) and of how the correctness of a model can be assessed by different validation criteria by M. Archer (ITQB Oeiras, Portugal). Evening lectures included two lectures on ribosomes by A. Liljas (Lund Univ., Sweden), overviews of automation at ESRF (G. Leonard) and of SPINE (K. Wilson).

During the entire course, a box to which specific 'burning questions' about crystallography could be submitted anonymously was available. These questions were later answered by the tutors in a special session. This proved to be very popular and gave valuable feedback to the tutors.

All participants were staying in the same hotel, which provided an excellent interactive environment. The City Council of Oeiras generously invited all participants to a dinner in the Fabrica de Pólvora a historic landmark of the region. Another evening was spent at a typical Portuguese restaurant enjoying regional cuisine and regional folk dances.

We thank the European Union and the IUCr for the generous support that made it possible to organize this second edition of this course on the fundamentals of crystallography. We are also grateful to the informatics staff of ITQB and especially to M. Mateus for efficient handling of course administration and logistics.

Maria Arménia Carrondo, Thomas R. Schneider, Organizers

MEETING REPORT

Micro- and mesoporous mineral phases

Mineralogical, crystallographic and technological aspects

Rome, Italy, December, 2004



The meeting, held at the Accademia Nazionale dei Lincei - Rome, Italy, December 6-7, 2004, was organized jointly by the Commission on Inorganic and Mineral Structures of the IUCr and the Nat'l Italian Accademy of Lincei, and covered recent advances in the field of micro- and mesoporous compounds. The meeting was organized by G. Ferraris, F. Calderazzo, S. Merlino and A. Mottana.

All sessions were held in a splendid hall of Palazzo Corsini, the magnificent venue of the Academy. After the opening ceremony, during which a brief account of the scope and activities of the IUCr was presented, the 6 oral sessions were devoted to the structural and crystal chemical aspects of porous systems, including their natural occurrence, possible synthesis, chemical-physical characterization, structure-property relationships, and uses as nanomaterials.

The meeting included 12 invited, 20 contributed presentations and 53 poster presentations; 98 participants from 20 different countries attended. We are grateful for the financial support from IUCr and other national and international institutions, associations and companies. Italy (local people were also involved in the organization) and Russia had the largest numbers of participants, but countries like Bulgaria, Iran, Rumania, Singapore, Turkey and Thailand were also represented. Delegates and contributions covered: crystallography, mineralogy, chemistry, materials sciences, physics, biology, and industrial research. The possibility of approaching different aspects of porous materials was highly appreciated by the participants, most of which were not crystallographers even if to some extent users of crystallographic methods.

Copies of the abstract book can be obtained free of charge by contacting delbuono@lincei.it. Twelve oral contributions are in press as volume 57 (same title as the meeting) of the *Reviews in Mineralogy and Geochemistry*. A number of other contributions will be published in a dedicated issue of the *European Journal of Mineralogy*.

Davide Viterbo and Giovanni Ferraris

MEETING REPORT

National seminar on crystallography

Gauhati University, India, January 2005



ICA President Dr. Krishan Lal speaking at the Inaugural Session of XXXIV National Seminar on Crystallography

The XXXIV National Seminar on Crystallography was held for the first time in the northeastern region of India at Gauhati U. on January 10-12, 2005. This remote region is geographically and ethnically different from most other parts of India and thus this meeting helped achieve the important objective of spreading crystallographic education and research in the seven Indian states of the region. As the seminar was held in the aftermath of the Great Asian Tsunami of December 26, 2004, attendance was reduced in the 136 presentations during oral and poster sessions. The topics covered all branches of crystallographic research and education. Macromolecular crystallography dominated the proceedings. J.K. Dattagupta (Saha Inst. of Nuclear Physics, Kolkata) delivered his keynote speech on plant proteins. Other areas that received due attention included the identification and structural characterization of new organic and metal-organic substances. The meeting held against the backdrop of the prediction of a big earthquake in Assam, the Indian state of which Guwahati is the capital city, brought interesting observations (apart from the scientific contents *per se*) from scientists of renowned Indian institutions including the Indian Inst. of Science, Bhabha Atomic Research Centre, the Indian Inst. of Technology, The U. of Madras, Indian Assn for the Cultivation of Science (IACS – Kolkata), Banares Hindu U. (BHU, Varanasi), All India Inst. of Medical Sciences and Nat'l Chemical Lab. (NCL, Pune).

The highlight of the seminar was an evening presentation 'On the Legacy of GN Ramachandran' by M. Vijayan that was followed by the screening of a beautifully produced VCD *Immortal Coils* on the life of G.N. Ramachandran and his work on collagen and the very lively annual meeting of the Indian Crystallographic Assn presided over by the well known materials physicist cum crystallographer Krishan Lal (Nat'l Physical Lab., New Delhi). A talk on crystallographic education was delivered by T.N. Guru Row (Indian Inst. of Science). Other speakers included V. Pattabhi (U. of Madras) who spoke on weak interactions, M.R.N. Murthy (Indian Inst. of Science) adroitly mixing little bits of crystallographic education with protein structure of microorganisms, and S. Mazumder (Bhabha Atomic Research Centre) talking on Small Angle Scattering. H.L. Duorah, former Vice-Chancellor of Gauhati U. and a well-regarded astrophysicist, delivered the Valedictory Address, which was inaugurated by the pioneering crystallographer-physicist of yesteryear, B. Chaudhuri (Professor Emeritus, Gauhati U.).

Birinchi Kumar Das, Convener

NOTICE

NMR crystallography

When the President of the IUCr gave the introduction to the 35th International School on Crystallography at Erice, Sicily, in June 2004, he listed particular divisions of the subject as X-ray Crystallography, Neutron Crystallography and Electron Crystallography. This list, whilst probably not intended to be exhaustive, is now rather obviously defective in not containing the increasingly important area of NMR crystallography.

NMR is an exceedingly important tool for chemical structure determination and also for the study of molecular-level mobility. It is accepted as by far the most powerful technique for such investigations for chemical compounds in the solution state. This situation arises from the fact that NMR spectra show exceedingly high resolution, thus distinguishing between atoms in closely similar chemical sites.

The situation is very different for solids, which, without the use of special techniques, generally give rise to broad unresolved resonances. Therefore, in the period 1955-1975 chemists largely ignored NMR of solids. However, the situation was revolutionised in 1976 by the development of the suite of techniques for ¹³C NMR (and subsequently for other nuclei) comprising cross-polarisation (CP), magic angle spinning (MAS) and high-power proton decoupling (HPPD). Since that date these techniques have become widely used and many refinements and developments have been produced. The result is that much crystallographic information can now be derived from NMR and the technique is increasingly important in this area.

NMR methods are sufficiently advanced that complete crystal structures have now been determined for the first time without other information. There is now truly a subject which may be called “NMR Crystallography”. This is generally complementary to diffraction crystallography, as demonstrated by a number of the above points. Unfortunately, NMR efforts in the investigation of crystallography have been very slow to be integrated with those of the rest of the crystallographic community, so that many “diffraction-based” crystallographers do not consider solid-state NMR as a natural part of their suite of techniques. Whilst it is mildly encouraging to see that the program for the Florence Congress this August contains sub-sections under two of the Congress main topics (though both, for some inexplicable reason, appear to be limited to macromolecules), these are the only mentions of NMR and there is nothing under the main topic number 01 “Instrumentation and Experimental Techniques”.

Perhaps now is the time to consider constituting a division of NMR crystallography within IUCr. Certainly a formal or semiformal link with the solid-state NMR community is desirable.

Robin K. Harris, University of Durham, UK

A few points about NMR and its potential applications to crystallography are as follows:

- NMR responds to the short-range environment of relevant atoms and is not directly influenced by long-range order.
- It can therefore be applied to amorphous materials as well as crystalline ones, though with broader lines for the former to encompass the variations in nuclear environments.
- It can be readily used to determine the chemical nature of a solid compound, including crystallographically important information such as conformation and tautomeric form.
- Chemical shifts give information about intermolecular interactions.
- Inter- and intra-molecular hydrogen-bond linkages can be identified.
- Information on crystallographic asymmetric units is especially readily available, usually merely by counting lines.
- Polymorphs are usually easily distinguished.

- Phase transitions can be monitored.
- Crystallographic disorder is detectable, and distinctions between spatial and temporal disorder can be made.
- Motions such as internal rotation and ring inversion can be detected and their rates obtained, even in cases of mutual exchange (e.g. 180° ringflips of phenyl groups).
- More general information about molecular-level mobility can be obtained by measurements of relaxation times.
- Measurement of dipolar coupling constants yields through-space inter-atomic (i.e. internuclear) distances, though these will be modulated by local mobility.
- NMR data can be used as restraints in carrying out full structure determination from powder diffraction data.
- Heterogeneous materials can be studied and selective spectra for particular domains obtained by the use of special pulse sequences.
- Intensities can be made quantitative (e.g. for polymorph ratios or crystallinity proportions).
- NMR is a multinuclear technique, each relevant isotope and element having its own specific frequency range.
- NMR experiments can be tailored to produce particular results by suitable choice of pulse sequences.

NOTICE

The Cambridge Crystallographic Data Centre

40 years of database development, software and research

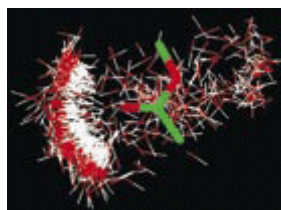
www.ccdc.cam.ac.uk

Beginnings



The CCDC was created to record crystal structures, and the Cambridge Structural Database was one of the first numerical databases created anywhere in the world. The CCDC dates from January 1, 1965, when David Watson joined Olga Kennard's research group in the Dept. of Chemistry at Cambridge U., UK. They began collecting references to organic and metal-organic crystal structures and began to encode bibliographic and numerical data in 'machine-readable' form. Subsequent CSD growth statistics suggest that if this work had not started then, it is doubtful if it would have started at all. But it did, and 40 years later the fully retrospective CSD contained 335,276 structures.

The CSD - then and now



Early progress was slow: computer technology was in its infancy and hardware was temperamental! Nevertheless, other group members were increasingly attracted to the new world of informatics, since crystallographer-programmers were needed to turn the vision into a reality. They created systems for logging, encoding and validating data, and today our scientific editors and their assistants are fully responsible for CSD creation and maintenance. Structure validation software was an early requirement, to detect local data entry mistakes and the typographical errors that occurred in some 10% of printed tables. Data acquisition itself has now completed its own 'electronification' from printed journal tables to electronic CIF depositions. The IUCr has itself played a key role in this essential transformation.



Former directors David Hartley and Olga Kennard join current director Frank Allen. *photo courtesy of Sarah Houlton, Chem@CamNewsletter*

An electronic bibliographic file was being regularly updated by 1970, and was published via the *Molecular Structures and Dimensions* book series, again with IUCr involvement. Meanwhile, the first 5,000 crystal structures were being validated and entered into a CSD data file. Finally, a chemical

connectivity file was created, thus enabling 2D and 3D substructure searching and adding tremendous value to the underlying crystal structure data. These three separate files were soon amalgamated into the present-day CSD.

Now, the CSD includes 335,276 crystal structures, and grew by nearly 29,000 structures in 2004. The size and complexity of structures has also increased steadily with time. The CCDC has excellent relationships with journals, and 84 titles now require electronic data deposition to the CCDC when a paper is submitted. These data enter the CSD when the paper is published, and the CCDC maintains a growing parallel archive of more than 160,000 of these initial 'raw' CIFs. Individual CIFs can be freely downloaded from this archive using a simple web form. The CCDC's enCIFer software, available for free download, is designed to help depositors create format-compliant CIFs for submission to journals and databases. Current CSD statistics, available on the website, refer primarily to published data, although the CSD now contains more than 3,000 *Private Communications*. Finally, the very large number of unpublished structures that languish in laboratory archives is surely a matter that must be addressed in the future.

Millions of lines of code

Software development has always been at the heart of CCDC activities, and we have run the gamut from FORTRAN II to our current object-oriented C++ environment. The CCDC develops three types of code: that which underpins CSD creation, that which forms part of the distributed CSD System, and applications software that uses crystal structure data to solve problems in structural chemistry and biology. CCDC software developers have been at the forefront in creating novel systems for 3D substructure searching, including searches for intermolecular interactions, and the statistical analysis of parameter distributions retrieved from the CSD.

Two new components of the distributed CSD System have been added since 1997. These are knowledge-based libraries of intramolecular geometry (Mogul) and intermolecular interactions (IsoStar). They provide click-of-a-button access to millions of individual pieces information that can be derived from the CSD (and PDB protein-ligand complexes in the case of IsoStar). Further development, and integration of structural knowledge with other software, is ongoing in both cases.

Recent years have also seen the CCDC diversify into developing specific software applications for rational drug design (GOLD, SuperStar, Relibase+) and structure solution from powder data (DASH). All of these products use crystal structure data from the CSD or PDB, and most are being developed through collaborations with industry and academia. The life sciences products, concentrating on protein-ligand interactions and protein-ligand docking, help solve difficult problems, and promote the value of small-molecule crystal structures to a wide audience. The CCDC continues to broaden its own horizons, by seeking new areas of science where structural data adds value to research and development activities.

CSD System releases

By the mid-1970s, the first version of the CSD System had been released to academics in the UK, USA, Japan and Italy. Many other countries formed academic National Affiliated Centres and access extended rapidly. The pharmaceutical and agrochemicals industries began to experiment with computational chemistry and modelling tools for rational molecular design, and the number of industrial subscribers began to rise during the 1980s. Early releases were on magnetic tape, and software was released as source code to be compiled under the user's local operating system. Today all that has changed, with just a few universal operating systems, CDs and internet downloads, click-of-a-button installers, and e-mail support desks.

1,200 applications papers

The first papers that made use of the CSD for fundamental research began to appear in the late 1970s. Inspired by the work of Hans-Beat Buergi and Jack Dunitz on structure correlation, there was a rapid

acceleration in this type of research from about 1980. A key issue was to improve database searching and develop a proper statistical basis for data analysis, so that improvements in CSD distributed software were often driven by current research needs. The CCDC itself has been heavily involved in this research effort, and has published applications papers covering both intramolecular and intermolecular topics. Tables of mean bond lengths ^[1,2] have jointly received more than 10,000 citations, while in the study of intermolecular interactions the CSD has provided tools for studying protein-ligand interactions, and played its part in the emergence of crystal engineering as a sub-discipline. One CCDC paper, which categorised short C-H...O interactions as true H-bonds ^[3], has received >1,000 citations and has re-shaped the global view of weaker interactions. The CCDC maintains a web accessible database of published product applications, and the 1,200 current entries chart the many and varied uses of the CSD. The CCDC is well represented with over 150 papers, but more than 1,000 other references indicate the truly international impact of CSD-based research.

The CCDC as an independent institution

The CCDC was grant-funded from 1965 until 1989, when it became an independent institution: a non-profit charitable Company Limited by Guarantee under English law. Thus, the CCDC must now be financially self-sufficient, and any surplus income must be used internally (e.g. for new equipment) or for specific charitable activities. Significant contributions are made to ensure CSD System access in developing countries, together with support for students and professional organisations. The CCDC's affairs are overseen by an international Board of Governors, eight eminent scientists who, in their turn, are responsible to UK Companies House and to the Charity Commissioners for England and Wales.

Our most valuable assets: staff and customers

The CCDC has expanded steadily, and now has 50 employees divided between database creation, product development, research, scientific and technical support, and administration. More than 250 people have worked at the CCDC, and each has left their mark on the organisation. The CCDC now has a worldwide customer base in academia and industry, and the 2,000 CSD System licenses were distributed across 56 countries in 2004. Customers and data depositors also leave their mark, through their constructive feedback on our efforts. The CCDC, our products, and ultimately all of our customers, have benefited enormously from these interactions.

We look forward to the next 40 years.

[1] *J.Chem.Soc. Perkin Trans.*, pp S1-S19, 1987.

[2] *J.Chem.Soc. Dalton Trans.*, pp S1-S83, 1989.

[3] *J. Amer. Chem. Soc.*, **104**, 5063-70, 1982.

REGIONAL NEWS

Crystallography in Russia

Computational mathematics and cybernetics at Moscow State University

Since the 1950s, research on the development of numerical methods and software for defining the structure of materials based on the data from diffraction experiments have been performed in the Inverse Problems Laboratory in the Computational Mathematics and Cybernetics Dept. of Moscow State University. Boris Shchedrin is head of the laboratory.

Within the last decade basic scientific efforts have concentrated on the following topics: the phase analysis of polycrystals; the numerical solution of autocorrelation functions; processing and interpretation of reflectometric data from thin multilayer organic films; and the development of numerical methods for interpretation of diffuse scattering from crystals with nanostructure inclusions.

The basic results are:

- Estimates of the agreement between spectra of probable phases in an alloy and the spectrum of the sample have been proposed and a dialogue for the intellectual phase analysis of polycrystals has been created^[1];
- On the basis of previous theoretical work effective algorithms for the interpretation of the Patterson function of monocrystals have been developed. The uniqueness of solution of the restoration problem for spherically symmetric particles and two-dimensional finite axial distribution has been proven^[2];
- Numerical methods and software packages for the restoration of structure of thin multilayer organic films from reflectometric data (small-angle scattering) have been developed;
- An effective multiresolution method for analysis of diffusive scattering from crystals with nanosized clusters has been developed^[3,4].

Work on the highlighted topics was conducted in collaboration with employees of the Institute of Crystallography of the Russian Academy of Science (The Structural Analysis Laboratory, led by V.I. Simonov and the Small-angle Scattering Laboratory, led by L.A. Fejgin).

Contact: B. Shchedrin (bshchedr@cs.msu.su)

[1] Burova E.M, Shchedrin B.M. A windows application: the program for qualitative phase analysis of polycrystalline mixtures. (2000). *Crystallography Report*, 45, 340-342.

[2] Shchedrin B.M. On the existence of solution in the inverse problems of the substance structure restoration on the diffractive data. (2000). *Applied Mathematics and Computer Science, Moscow: Max - press*. N. 6, 67-71.

[3] Andrushevsky N.M, Shchedrin B.M., Malahova L.F., Simonov V. I. Diffusive scattering from crystals with dot defects. (2002). *Crystallography (Russia)*, V. 47, N. 3, 518-521.

[4] Andrushevsky N.M., Shchedrin B.M., Simonov V.I. Restoring algorithm of atomic structure of nanosized inclusions in crystals on the base of diffuse scattering of X-rays or neutrons data. (2004). *Crystallography (Russia)*.

OBITUARY

Mario Nardelli (1922-2004)



Mario Nardelli died at home in Parma, Italy on September 24 2004 in his 82nd year after 58 years increasingly and fruitfully dedicated to research and teaching. He was amongst the leading crystallographers in the world and one of the pioneers in the field of structural chemistry by single crystal X-ray diffraction in Italy and leaves a school of Structural Chemistry in Parma well known among the crystallographers of the world.

What follows is a portrait of the scientist and of the man, outlined by those who were close to him, but we believe that everybody who knew Mario will share our memories of him.

Mario Nardelli was born in Parma on January 6, 1922; he was educated at the classical lyceum of Genova until 1941. He then moved back to Parma and in March 1946 he obtained his degree in Chemistry *summa cum laude* at the University of Parma.

He started his academic career in 1946, as an Assistant Professor, under the guidance of Adolfo Ferrari who stimulated the initial interest of this bright young researcher in the analysis of crystal structures of inorganic salts by X-ray diffraction methods. In 1950, he was awarded the Italian National Special Prize for "Scientific Endeavour".

In 1963, thanks to his intense and fruitful research activity, Mario Nardelli was appointed to the Chair of Structural Chemistry at the Faculty of Mathematics Physical and Natural Sciences of the University of Parma. In 1967, he succeeded Adolfo Ferrari as Full Professor of general and inorganic chemistry and maintained this academic position until October 31, 1996, when the Italian Ministry for University and Scientific and Technological Research awarded him the title of Professor Emeritus.

Mario Nardelli was the head of the Institute of Structural Chemistry at the University of Parma and founded a school of crystallography, held in high national and international esteem. From 1979 to 1992, he also directed the Centro di Studio per la Strutturistica Diffattometrica of the Italian National Research Council (CNR) in Parma.

He held many academic and institutional positions, Dean of the Faculty of Pharmacy, member of the Administrative Council of the University of Parma, President of the Italian Crystallographic Assn. He was a member of the National Italian Commission of the National Research Council (1969 to 1975). In 1976 he was awarded the gold medal for "Meritorius Persons in School, Culture and Arts".

In the early sixties, to promote research in structural chemistry in Parma, Prof. Nardelli worked on the the foundation of the first computing center at the University of Parma of which he was director for more than twenty years; at the same time he was one of the leaders of CINECA (National Center for Supercomputing and University Services), one of the foremost computing centers in Europe. Mario foresaw the importance of a knowledge of computing science for young generations from the very beginning, in 1966 he promoted (for the first time in Italy) the teaching of computer programming in the chemistry degree at the University of Parma.

He was a member of the Data Commission of the IUCr (1975 to 1981) and a member of the IUCr Executive Committee (1981 to 1993). In 1987 he was elected President of the IUCr, and from 1990 to 1993 he represented the Union at the International Council of Scientific Unions.

He made an important contribution to the growth and diffusion of crystallography in the world when, in 1972, he founded the Journal *Crystal Structure Communication* in which the data, reported in structural papers, were submitted for the first time to an automatic check prior to publication.

This journal was incorporated into *Acta Crystallographica* Sect. C in 1983 and the automatic check of crystal structures was extended to all the papers published in journals where crystal structures are reported.

From 1981 to 1988, and from 1991 till his departure, he was Co-editor of *Acta Crystallographica* B, C and E and, in this capacity, he dedicated most of his time to checking many of the papers submitted to the journal personally; to many authors, he not only gave advice on mistakes that had been made, but also provided an accurate analysis of the source of the errors and the exact values, calculated by himself.

Mario was highly rigorous in his scientific activity, and dedicated much effort to finding methods for calculating the reliability of reported data, including estimated standard deviations. For this reason, he devoted part of his time to writing a series of crystallographic computing programs, made freely available to the crystallographic community.

But, throughout this intense range of activities, he always remained attracted to every scientific question, and anyone with an intriguing problem always found his door open.

Mario Nardelli constantly stimulated our interest in chemical crystallography but we were always free to choose our research lines and to decide how to organize our activities even if he was always ready, when asked, to give us help and advice.

He always kept a humble attitude, without prejudice with regards to science and colleagues. Most of us remember when he, already famous in the world of crystallographers, attended (with some of us as the teachers) as an ordinary “student” the Italian Schools of Crystallography, a traditional school mainly organized for young researchers who were taking their first steps in crystallography, because, as he always used to say “there is always occasion to learn”.

We now receive this scientific and moral inheritance and it will be our duty to transfer the human and scientific lessons of Mario Nardelli to the new generations of young researchers.

His fellows at the University of Parma

OBITUARY

Federico Bedarida (1924-2004)

Federico Bedarida, Professor in Crystallography at Genoa University until 1999, died December 12, 2004 at the age of 80.

From the beginning of his academic career, “Beda” (to friends) gave an original and quite anomalous touch to his style of Italian Crystallography.

His lifelong interest in crystal surface investigations arose from the Tolansky papers on optical interferometry. At the beginning of the 1960s he spent a year in the Physics Dept. of London University (Holloway College) where he studied the microtopography of crystal surfaces under the guidance of S. Tolansky. He became an expert in new optical techniques, such as double beam interferometry and the analysis of the interference fringes of equal chromatic order and light profiles. In the 1970s, Bedarida and his Genoa team (C. Pontiggia, L. Zefiro and successively P. Boccacci) refined these techniques by applying holographic interferometry to reflection microscopy. They succeeded in depth mapping of a crystal surface relief by the multiple wavelength holographic technique.

He was fascinated by crystals as “...entities which bring and loose life from the surrounding through their surfaces...”. Frequent contacts with the people of Kern’s School in Marseille, with P. Hartman in Leiden, H. Arendt and E. Kaldis (Zürich) urged him toward crystal growth and, in particular, to characterization of the state of the solution around a growing or dissolving crystal.

During the 1980s he measured the concentration field in a supersaturated solution near growing crystal by means of multidirectional interferometry.

In order to check crystal growth in a microgravitational environment in collaboration with ESA, ASI and Alenia Spazio, the prototype of a compact optical tomograph was designed making use of optical fibers.

In the meanwhile, G. Dall’Aglia and E. Piano joined the research group. Using a new home made phase measurement device (from optical diffraction) they obtained very localized information down to 20 microns from the crystal/solution interface.

He was sensitive to all problems concerning real crystals and he devoted his energies to opening up new horizons in Italian Crystallography. He was a co-founder of the Italian Crystal Growth Association (AIC) and promoted the first Italian schools on crystal growth, in 1977, along with other international schools on crystal growth in Erice (1975, 1981, 1987).

This plain man of great culture, endowed with that rarest thing which is common sense, created an agreeable work environment for all those who had the privilege of collaborating with him.

Dino Aquilano

OBITUARY

Erwin Felix Lewy-Bertaut (1913-2003)



Erwin Felix Lewy-Bertaut, member of the French Academie des Sciences, former Directeur de l'Institut de Cristallographie à Grenoble (France) died in Grenoble on November 6, 2003.

Erwin Lewy was born as a member of a cultivated Jewish family in the small town of Leobschütz in the year 1913. Leobschütz was situated in Upper Silesia which was then part of the German Empire. The place was, however, very close to the border of Austrian-Hungarian Empire and is now situated in Poland near to the Polish-Slovakian border. His father was a professor of classical languages (Latin and Greek) in the local Gymnasium and Erwin Lewy first enrolled in the University of Freiburg and studied law and philosophy (with Heidegger). As a consequence of the political change in Germany he emigrated to France in 1933. He arrived at Bordeaux and changed to science. He once told me that after the events in Germany he was unable to follow the humanitarian ideas of his youth and he decided to concentrate on a subject far from any ideology. He joined the French Army in 1939 interrupting his PhD thesis at Bordeaux and after the French defeat he received a temporary identity card under the name Felix Bertaut. During the occupation he was first in the southern part of France controlled by the Vichy government but joined then the Laboratoire Central des Poudres in Paris where he came in contact with crystallography. Finally after some dangerous situations with police controls he joined the team of professor Louis Néel in Grenoble. Under the guidance of Néel the Laboratoire d'Electrostatique et de Physique du Métal (LEPM) was created as the first CNRS institute outside Paris.

Erwin Lewy obtained a CNRS research fellowship as Felix Bertaut and choose a new thesis subject "Study of size statistical distribution of iron grains by means of X-rays". His thesis was in close relation with the main subject of Néel, magnetism, and it was also very modern in the sense of industrial application and nanotechnology. The thesis was defended in 1949 and the method developed by Bertaut is still a reference in powder diffraction. Inspired by the first neutron diffraction experiments on antiferromagnetic MnO Néel and Bertaut decided to establish neutron diffraction in Grenoble. Bertaut went to the United States several times to study new techniques in Brookhaven with Corliss and Hastings. After the decision of the French government to install an atomic research center in Grenoble (C.E.N.G.) under the direction of Néel, Bertaut created the "Diffraction Neutronique" laboratory within the CENG which he directed from 1958 to 1976. A unique discovery related with the name of Bertaut (together with Francis Forrat and René Pauthenet) was the synthesis of rare earth iron garnet ferrites and the detailed study of their magnetic structure and properties.

The LEPM increased in size over the years and was split in 1971 into several independent laboratories. Among them was the Laboratoire de Cristallographie headed by Felix Bertaut from 1971 to 1982. In 1963 I joined his research group as the first German student and it took me some time to realize his German origin. But I was then deeply impressed to observe the many contacts which he had already established with German laboratories during the fifties despite the destiny of his family. Many foreign visitors (established scientists as well as PhD-students) created a lively international atmosphere. This experience has definitely influenced me to open my own laboratory to guests from abroad. The idea of a high flux neutron reactor as a common German-French project was launched in Grenoble during the first International Conference on Neutron Scattering in 1963. It had been promoted by Néel and Bertaut and led in 1967 to the High Flux Research reactor at the ILL: The name of the Institut Laue-Langevin

combines scattering and crystallography with magnetism in a convincing way. Now the German-French nucleus has become a real European institution and was the main reason to construct the European Synchrotron Radiation Facility (ESRF) at Grenoble.

Prof. Bertaut contributed to various areas of crystallography. Powder diffraction and grain size distribution have already been mentioned. His share in establishing “Direct Methods” has partially been ignored as his main articles were published in French during the fifties. The definition of the concept of Group Theory to predict magnetic structures was, however, applied in many neutron diffraction laboratories around the world. Due to his broad education in chemistry, physics and mathematics he always combined synthesis of new materials (mainly oxides and sulfides) with their physical (mainly magnetic) properties. He was a member of IUCr committees and the Executive Committee from 1975-1981. Awarded several prizes and acknowledged as Professor Honoris Causa by Universities in Sweden and Germany, he became a full member of the French Academie of Sciences in 1979.

Erwin Felix Lewy Bertaut was “un savant pas seulement un scientifique” Furthermore he was a humanist in the classical sense of the world, a witness of the twentieth century, a convinced European, a great crystallographer and a remarkable man.

Hartmut Fuess

OBITUARY

Ramachandran Srinivasan (1933-2004)

Ramachandran Srinivasan, a well-known crystallographer, passed away on September 19, 2004. He had been associated with the Dept. of Crystallography and Biophysics, University of Madras for the past four decades. He was respected in India and abroad for his contributions to crystallography.

He was born on July 5, 1933 at Nannilam in Tamilnadu. His B.Sc. (Hon.) (1953) and M.Sc degrees (1954) were from the University of Madras. After completing his M.Sc. with distinction he joined the physics dept. of the University of Madras for a Ph.D. degree in X-ray Crystallography, under the guidance of G.N. Ramachandran.

Srinivasan was associated with G.N. Ramachandran during an exciting and productive period of theoretical crystallography and biophysics in India. In 1962 he visited the Cavendish Laboratory, University of Cambridge under a Commonwealth Fellowship Program. He became a full professor in 1964, one of the youngest professors in the history of the University of Madras. He became senior professor in the year 1972. He was the head of the Dept. of Crystallography and Biophysics from 1969 until his retirement in 1994. He was a visiting scientist at the Dept. of Biological Sciences, Purdue University in 1968 and he used this opportunity to write his famous book on "Fourier methods in crystallography", which was co-authored by G.N. Ramachandran.

His research interests included theoretical crystallography, polytypism, structural biophysics, nuclear magnetic resonance, gemology and musicology. He published over 200 papers in national and international journals. He edited or wrote nine books and monographs.

He had a deep knowledge of Fourier transform theory and he used this knowledge to develop many new methods for recovering information (atomic sites) from imperfect electron density maps. He, along with G.N. Ramachandran and S. Parthasarathy, developed special Patterson and Fourier syntheses for use in crystal structure analysis. They showed that the phase angles have an overwhelming importance in revealing structure and that amplitudes play only a secondary role. His group proposed several weighting functions for the improvement of Fourier maps. These results are summarized in the monograph entitled "Fourier Methods in Crystallography" published in 1970 by John Wiley and Sons.

He was a pioneer in the application of statistical analysis of interactions to the solution of crystallographic problems. Useful results obtained by him included a test for centrosymmetry and derivation a probability distribution of structure factors from a pair of related crystals.

The probability distribution of Bijvoet differences, the statistical treatment of unobserved reflections in least squares refinement, and statistical tests for isomorphism in crystals are some of his other contributions to theoretical crystallography. He published 80 papers in the area of crystallographic statistics and a monograph with his colleague S.Parthasarathy, entitled "Some statistical applications in X-ray crystallography".

He made significant contributions to the theory of anomalous dispersion. He was in one of the early groups of scientists who worked out the application of anomalous scattering to solve the phase problem. He pointed out that phases could be determined using multiple wavelength anomalous techniques as well as single wavelength anomalous scattering. He suggested that the phenomenon of isomorphism

could be simulated with a single crystal by making use of the anomalous dispersion effect. This work led to a review article on “Applications of X-ray anomalous scattering in structural studies” in *Advances in Structural Research by Diffraction Methods* (1972).

In the latter part of his career, he concentrated on structural biophysics. He proposed several new methods for characterization of biopolymers. The earlier method proposed by G.N. Ramachandran used two parameters, ϕ and ψ , for characterizing a biopolymer. Srinivasan reduced this to one parameter and carried out extensive analysis of protein data based on this idea. He introduced a virtual bond concept for biopolymer characterization.

Srinivasan developed a solid state NMR laboratory from scratch and constructed a NMR spectrometer with the help of his students. His main contribution in this area was on line shape analysis using truncated moments, which finds use in motional studies in solid state NMR.

Srinivasan was a good administrator and commanded respect from his colleagues and subordinates. He steered the research program of the department for more than two decades after G.N. Ramachandran left the University of Madras. He maintained the eminence of the department and attracted significant funding from various agencies.

He was an elected fellow of the Indian Academy of Sciences (1968), Indian National Science Academy and Institute of Physics (London). He was a founding member of Tamil Nadu Academy of Sciences, and a committee member of the IUCr Teaching Commission, National Committee for Crystallography and the Indian Biophysical Society. He leaves behind a host of students, colleagues and friends whose lives he enriched for the past four decades. All will cherish his memory and his work will continue to inspire crystallographers the world over.

Vasantha Pattabhi