

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



The meeting of the IUCr Executive Committee this year was held August 3-4 in Leuven, Belgium. I would like to highlight three important decisions.

The first decision concerns a new initiative on how to invite developing countries to become members of the IUCr. The number of member countries or Adhering Bodies of the IUCr is only 39 or 40, respectively. Many countries are members of the Regional Associates (ACA, AsCA and ECA) but not members of the IUCr. This is primarily because members of the IUCr are required by the Statutes to pay a subscription fee. Although the fee for Category I is just CHF 1,000 (about USD 800) per year, the payment is not so easy for National Associations with small numbers of members. I know several African, Central and South American or Asian countries in which there are only a few crystallographers. According to the new system, the IUCr strongly recommends crystallographers in such countries to form a country group and to establish a single Adhering Body to become a member of the IUCr. The subscription fee should be divided among the countries making the group. The Executive Committee expects more than one Adhering Body will be formed in this way in the area of each Regional Associate. Each country in the group would have the same rights as ordinary member countries except for the voting rights in the General Assembly, which depends on the Category of the Adherence. We hope that more than 20 countries will become new members of the IUCr in the next General Assembly following adoption of this system. The IUCr will offer a licence to one or more institutions in such countries to access IUCr online journals at a very low price. The IUCr believes that in this way new crystallographic initiatives will be able to start in such developing countries.

The second decision is that *Acta Crystallographica* Section E should be changed to be open access by 2008. Since this online-only journal was launched, the number of submitted manuscripts has been increasing exponentially. This is a delightful and successful event for the IUCr. However, the editorial work to make the journal has become huge. From a financial point of view, a serious crisis will arise in the near future if nothing is done. To avoid the crisis, it is reasonable to ask authors to pay to make it possible for everybody to read *Acta Crystallographica* E freely without a subscription - that is, the open access system. The submission fee is expected to be modest and only payable on acceptance. The detailed procedure is in preparation, including a provision for developing countries.

The third decision is a small change of the election procedure for IUCr officers. At the last General Assembly in Florence, there were many discussions by the delegates of the National Committees concerning the election procedure. The Executive Committee has considered the Statutes and By-Laws in detail and noted that it is possible to change the nomination procedure in order to encourage timely nominations from the National Committees without changing the present Statutes and By-Laws. The revised procedure is that following initial consultation with the National Committees (as is present practice) the Executive Committee will nominate one or two candidates for each position. Once they have been informed of these nominations, Adhering Bodies that wish to make further nominations will be asked to form a group of Adhering Bodies representing more than six voting rights in order to nominate additional candidates one month before the General Assembly.

The information concerning these nominees will be sent to all the National Committees before the General Assembly. The Executive Committee expects that this will provide time to enable sufficient discussion within each National Committee before the General Assembly meets. Of course, the present

deadline of 36 hours specified in the By-Laws for nominations by delegates will still be applicable. The Executive Committee always wants to do the best for the IUCr by accepting the proposals from the National Committees.

These decisions will be sent to all National Committees in the near future. The Executive Committee heartily welcomes constructive opinions not only from National Committees of member countries but also from non-member countries.

Yuji Ohashi, yohashi@spring8.or.jp

REGIONAL NEWS

Message from the new President of the ECA



John R Helliwell

Dear Colleagues,

It is a great honour for me to have been elected the President of the European Crystallographic Association (ECA) for the coming 3 years.

With this letter, I would like to initiate a review, and in depth discussion, of a long term strategy of development of the ECA. The ECA not only runs outstanding ECM conferences, but sponsors the prestigious Max Perutz Prize Lectures, has a very informative website (www.ecanews.org/) and is one of the three regional affiliates of the IUCr. It is now possible for individual members to join the ECA for a 5 year period for only 50 Euros using a credit card. A principal benefit of being a member is a reduced registration fee for the ECM. Membership dues help the ECA build a reserve to support student attendance at ECM and other crystallographic meetings. New members contribute to securing both a firmer foundation for the ECA and an opportunity to expand activities. An endowed Lecture prize fund has been set up for outstanding young crystallographers to present their 'Lewy-Bertaut Prize' Lecture (jointly with the European Neutron Scattering Association (ENSA) at the ECM). This, and the Max Perutz Prize and Lecture, continue to rely on annual contribution from individual members and commercial suppliers of crystallographic equipment and supplies, to whom we are very grateful. Dues from an expanded membership would secure additional support for these prize funds. Most importantly the ECA also needs to help provide financial assistance to young scientists and other colleagues in financial difficulties to attend our ECMs. National crystallographic associations that affiliate its members to the ECA are another important income stream. There are 29 national i.e. country members and 5 observer countries. Overall our total official number of members is approx 900. Since the total number of crystallographers in Europe is estimated at 4000 we are missing many potential members! Tell your friends about the ECA and how to join (see www.ecanews.org/membership.htm).

I invite you to email me your suggestions of how we can improve and/or expand our activities. One idea for discussion is to have satellite sessions at our ECMs for skills enhancement and training (e.g. how to use the latest software packages). This is also known as Continuous Professional Development. Another idea is that, rather than a paper printed newsletter, we have an "ECA e-Newsletter" with all articles and letters being sent to our webmaster, Massimo Nespolo (massimo.nespolo@lcm3b.uhp-nancy.fr). This will ensure a regular flow of information and news. I don't want to detract from the *IUCr Newsletter* content from Europe, but I feel sure that we have plenty of other news and views, that can't find outlet in the inevitably limited number of printed pages of the *IUCr Newsletter*.

It is a happy coincidence that I am writing this just when the IUCr Journals have won the Association of Learned Society Publishers ('ALSP') Publishing Innovation Award for its leadership in scientific publishing linking the data on which a publication rests to the detailed text. On behalf of the whole ECA I

congratulate the IUCr Journals in Chester on this terrific achievement as a, now, widely recognised leading innovator in science publishing.

In my next quarterly contribution to the ECA website, in December, I will report on progress with the ECM24 in Marrakech under the hard working Chairmanship of Abdelmalek Thalal and describe the background to agenda items coming up for discussion at the next ECA Executive Committee (whose members are listed at www.ecanews.org/conductors.htm) meeting to be held in Manchester in mid February 2007.

John R Helliwell , john.helliwell@manchester.ac.uk

NOTICE

A new IUCr commission on XAFS



Alfons Molenbroek, Chair of the Commission on XAFS

The new “Commission on XAFS” was officially endorsed by the General Assembly at the IUCr2005 Florence Congress. The members of the Commission for the next triennium are Kiyotaka Asakura (Japan), Isabella Ascone (Italy and France), Federico Boscherini (Italy), Maria-Ondina Figueiredo (Portugal), Britt Hedman (USA), Elisabeth Holub-Krappe (Germany), Joaquin Garcia-Ruiz (Spain), Alain Michalowicz (France) and Alfons Molenbroek (Denmark, chair). Samar Hasnain continued as a consultant for the Commission.

The main goal for the Commission will be to promote XAFS in the crystallographic community. At the Florence Congress, a successful microsymposium on “Combined XAS and XRD techniques in physics, chemistry and material science” was organized by Settimio Mobilio and Joaquin Garcia-Ruiz.

A website (www.iucr.org/iucr-top/iucr/cxafs.html) has been developed and contacts with the International XAFS Society (IXS) are being strengthened. Some of the members of this Commission also sit on other commissions and they are eager to improve relations for the benefit of both the XAFS and the crystallographic communities. The Commission might be involved in the support of workshops and summer schools.

Some Commission members met again at the 13th Int’l Conference on X-Ray Absorption Fine Structure (XAFS-XIII) held at the Stanford (www-ssrl.slac.stanford.edu/xafs13) on July 9-14, 2006. The third BioXAS Study Weekend was held at the new synchrotron radiation center SOLEIL, in France, close to Paris (www.synchrotron-soleil.fr) on August 10-12, 2007 as a satellite meeting of the 9th International Conference on Biology and Synchrotron Radiation (BSR2007).

Future activities might include (re-)addressing the tough parts of XAFS (definitions, data collection and analysis procedures).

Alfons Molenbroek and Isabella Ascone

NOTICE

Crystallographic teaching commission newsletter



Lachlan Cranswick

The first edition of the IUCr Teaching Commission newsletter (No. 1, June 2006) is available on-line as an Adobe Acrobat PDF file (www.iucr.org/iucr-top/comm/cteach/newsletters/june2006)

The theme of this edition is "Teaching Crystallographic Fundamentals". (This Issue's Editor is Lachlan Cranswick) Articles in the first issue include:

- IUCr Commission on Crystallographic Teaching
- Siena 2006 : IUCr School on Basic Crystallography
- Einstein's tongue for teaching crystallography to biologists - *Philippe Dumas, Julien Vanwinsberghe and Vincent Cura*
- Crystallography Education and Training in the United States - *Katherine A. Kantardjieff*
- Crystallographic Teaching in Pakistan - *Zia Khan*
- A Guided Tour in Fourier Space - *Fokke Tuinstra*
- The British Crystallographic Association Intensive Courses in X-ray Structural Analysis - *David Watkin*
- Teaching of the Fundamentals of Crystallography - *Dieter Schwarzenbach*
- Teaching Crystallography and Related Subjects at Novosibirsk State University, Russia - *Elena Boldyreva*
- Crystallographic Teaching at the Laboratory of Inorganic Crystal Chemistry at Moscow State University, Russia - *Evgeny Antipov*
- M.Sc. Crystallography at Birkbeck College, University of London, UK - *Alan L. Mackay*

Addendum 1: reprint of webpages containing the (now defunct) Birkbeck College M.Sc. Crystallography Course Syllabus in its final form (taken from Jeremy Cockcroft's website)

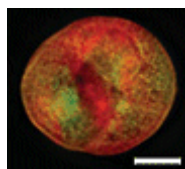
Addendum 2: mid 1950's (rejected) submission on crystallography by J.D. Bernal et al to the Encyclopaedia Britannica. The article was rejected as too long but it embodied the syllabus and intention of the Birkbeck College M.Sc. course in crystallography.

Call for Contributions to the Next Teaching Commission Newsletter: Providing there is enough interest, the second issue of the Teaching Commission Newsletter is expected to appear around June of 2007 with the primary theme to be determined. If no-one is else is co-opted, the newsletter will be edited by Lachlan Cranswick. Contributions would be also greatly appreciated on matters of general interest to the crystallographic teaching community. Please send articles and suggestions directly to the editor, Lachlan M.D. Cranswick (lachlan.cranswick@nrc.gc.ca , <http://neutron.nrc.gc.ca/peep.html#cranswick>).

IUCR JOURNALS NEWS

Reconstruction of a yeast cell from X-ray diffraction data

***Acta Cryst.* (2006). A62, 248-261 [doi.org/10.1107/S0108767306016515]**



Reconstructed yeast cell image (1 micron scale bar). Hue represents the phase, and brightness the amplitude, of the X-ray exit wave.

Diffraction microscopy (also called coherent diffractive imaging) extends traditional crystallography to the study of non-periodic objects. In this article we present a two-dimensional reconstruction of the image of an unstained yeast cell from its soft X-ray diffraction pattern. We place particular emphasis on algorithmic strategies that deliver reproducible results in the presence of noise and missing data. We also present a method to determine the effective resolution of images reconstructed by this technique.

P. Thibault, V. Elser, C. Jacobsen, D. Shapiro and D. Sayre

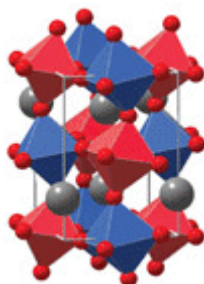
IUCR JOURNALS NEWS

Structure determination of $A_2M_3+TaO_6$ and $A_2M_3+NbO_6$ ordered perovskites: octahedral tilting and pseudosymmetry; Structure prediction of ordered and disordered multiple octahedral cation perovskites using SPuDS

Structure determination of $A_2M^{3+}TaO_6$ and $A_2M^{3+}NbO_6$ ordered perovskites: octahedral tilting and pseudosymmetry; Structure prediction of ordered and disordered multiple octahedral cation perovskites using SPuDS

Acta Cryst. (2006). B62, 384–396 [doi.org/10.1107/S0108768106002448];

Acta Cryst. (2006). B62, 397–410 [doi.org/10.1107/S010876810600262X]



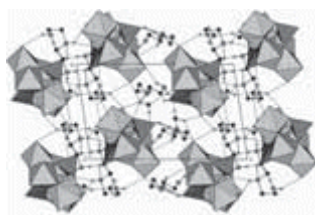
Although simple, the perovskite structure is also very flexible. The distortions that result from this flexibility are responsible for changes in physical properties that are of wide ranging importance. These two articles explore octahedral tilting distortions in perovskites from two perspectives. The first paper examines the challenges associated with accurate structure determination when the unit-cell dimensions remain highly pseudosymmetric. The second paper examines octahedral tilting in $A_2MM'O_6$ ordered perovskites and discusses the accuracy of the program SPuDS in predicting structures of ordered perovskites.

P.W. Barnes, M.W. Lufaso and P.M. Woodward; M.W. Lufaso, P.W. Barnes and P.M. Woodward

Bis(iminodiethylenediammonium) di- μ_5 -hydrogenphosphato-pentamolybdate(VI) tetrahydrate

Bis(iminodiethylenediammonium) di- μ_5 -hydrogenphosphato-pentamolybdate(VI) tetrahydrate

Acta Cryst. (2006). C62, m355-m357 [doi.org/10.1107/S0108270106023092];



A packing view along the b axis, showing the arrangement of the $[\text{Mo}_5\text{O}_{15}(\text{HPO}_4)_2]^{4-}$ clusters (polyhedra), the $(\text{H}_2\text{tren})^{2+}$ cations and the lattice water molecules in the crystal structure.

The crystal structure of $(\text{C}_4\text{H}_{15}\text{N}_3)_2[\text{Mo}_5\text{O}_{15}(\text{HPO}_4)_2] \cdot 4\text{H}_2\text{O}$ is made up of $[\text{Mo}_5\text{O}_{15}(\text{HPO}_4)_2]^{4-}$ anions, $\text{C}_4\text{H}_{15}\text{N}_3^{2+}$ cations and lattice water molecules. The $[\text{Mo}_5\text{O}_{15}(\text{HPO}_4)_2]^{4-}$ cluster, with approximate C_2 symmetry, can be considered as a ring formed by five distorted edge- and corner-sharing MoO_6 octahedra, capped on both poles by a hydrophosphate tetrahedron. There exist $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds between the organic components and the clusters.

Feng Geng, Guo-Hua Han and Bi-Zhou Lin

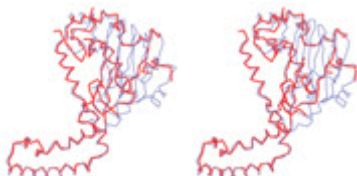
IUCR JOURNALS NEWS

The Buccaneer software for automated model building. 1. Tracing protein chains

The *Buccaneer* software for automated model building.

1. Tracing protein chains

***Acta Cryst.* (2006). D62, 1002-1011 [doi.org/10.1107/S0907444906022116]**



Buccaneer model and true structure from a 3.2 Å electron density map.

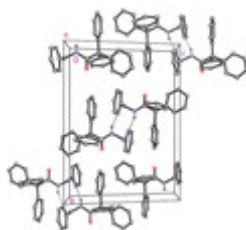
The manual fitting of an atomic model into a 3-d electron density map is a time consuming process, which is being automated by a number of projects. A new technique is described to identify likely candidate C α positions and then grow these into connected protein chains. Instead of relying on specific features observed in density maps at a particular resolution, the program generates a problem specific statistical target for finding C α positions in maps matching the map to be interpreted.

K. Cowtan

IUCR JOURNALS NEWS

2,2,2-Triphenyl-N-(2-pyridylmethyl)acetamide

***Acta Cryst.* 2006. E62, o3339–o3340 [doi.org/10.1107/S1600536806026109]**



While pyridyl amide ligands possess varied and versatile coordination properties with transition metal ions, they also display interesting hydrogen bonding characteristics. This report, along with its preceding companion report (*Acta Cryst.* 2006, **E62**, o3337), illustrates the importance of steric bulk in determining the type and extent of hydrogen bonding observed between pyridyl amide molecules. Hydrogen bonding in the less bulky 2-phenyl-*N*-(2-pyridylmethyl)acetamide gives rise to one-dimensional chains while hydrogen bonding in the more bulky 2,2,2-triphenyl-*N*-(2-pyridylmethyl)acetamide results in the formation of dimeric pairs.

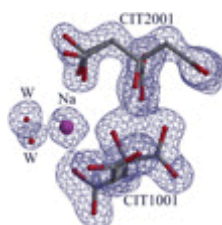
L.R. Whiteaker, U. Pal Chaudhuri, D.R. Powell and R.P. Houser

IUCR JOURNALS NEWS

The molecular structure of Rv2074, a probable pyridoxine 5'-phosphate oxidase from *Mycobacterium tuberculosis*, at 1.6 Å resolution

The molecular structure of Rv2074, a probable pyridoxine 5'-phosphate oxidase from *Mycobacterium tuberculosis*, at 1.6 Å resolution

Acta Cryst. (2006). F62, 735–742 [doi.org/10.1107/S1744309106025012]



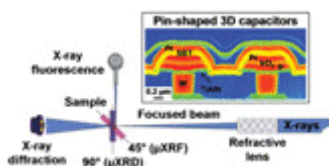
The $2|F_O|-|F_C|$ electron-density map (blue) contoured at the 1σ level, showing two citric acid molecules bound in the active site of Rv2074. The citrate carbon and oxygen atoms are shown in grey and red colors, respectively. Also shown are the sodium atom (magenta) and two coordinating water molecules (red).

In an attempt to predict the biological functions of conserved hypothetical proteins among the *Actinomycetes* subgroup of bacteria from their three-dimensional structures, the crystal structure of Rv2074 from *Mycobacterium tuberculosis* (Mtb) was determined. Rv2074 is a dimer in the crystals; each monomer folds into a six-stranded antiparallel β -barrel flanked by two α -helices. Owing to its extensive structural similarity with Mtb Rv1155 and to the *E. coli* and human pyridoxine 5'-phosphate oxidases, Rv2074 may possibly be involved in the final step in the biosynthesis of pyridoxal 5'-phosphate (PLP, vitamin B₆). Two citric acid molecules are bound fortuitously to the proposed active site of Rv2074.

Bichitra K. Biswal, Karolyn Au, Maia M. Cherney, Craig Garen and Michael N.G. James

Microstructural analysis of integrated pin-shaped two-dimensional and three-dimensional ferroelectric capacitors from micro-focused synchrotron X-ray techniques

J. Appl. Cryst. (2006). 39, 376–384 [doi.org/10.1107/S002188980601082X]



Schematic of the experimental setup for μ XRF and μ XRD. The top right of the figure presents a TEM cross section of 3D capacitors showing the ferroelectric SBT film deposited on an etched bottom electrode stack Pt/IrO₂/Ir/TiAlN on top of a W-plug.

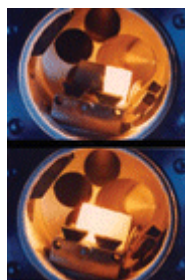
Future developments of Ferroelectric Random Access Memories (FeRAM) require integration of 3-dimensional (3D) ferroelectric capacitors in the memory architecture. Considering the critical role of the storage capacitor on the memory reliability, it is of particular interest to analyze the microstructural characteristics of the ferroelectric capacitors after the fabrication steps. The present novel approach consisting in the association of micro-focused synchrotron X-ray fluorescence (μ XRF) and diffraction (μ XRD) has been demonstrated as an efficient non-destructive diagnostic tool enabling relevant analysis of pin-shaped 3-dimensional ferroelectric capacitors.

N. Menou, Ch. Muller, L. Goux, R. Barrett, J.G. Lisoni, M. Schwitters and D.J. Wouters

IUCR JOURNALS NEWS

Combustion front dynamics in the combustion synthesis of refractory metal carbides and di-borides using time-resolved X-ray diffraction

J. Synchrotron Rad. (2006). **13**, 326-335 [doi.org/10.1107/S0909049506020796]



Time lapsed photos for the combustion synthesis of $\text{Zr} + \text{C} \rightarrow \text{ZrC}$ in the diffraction-reaction chamber. Top: half-way through the combustion after ignition with the tungsten coil powered off. Bottom: at completion of combustion. The combustion front was moving from right to left at a velocity of 5.8 mm s^{-1} as recorded with a video camera.

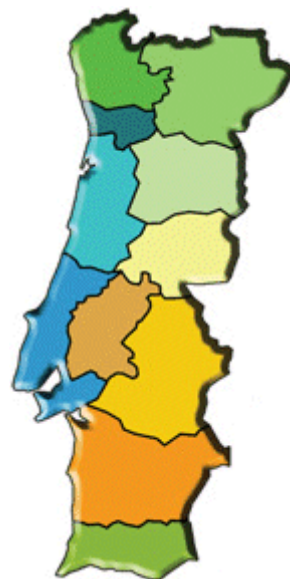
Synchrotron time-resolved diffraction was used to elucidate the combustion dynamics of refractory metal carbides and diborides (Figure). The combustions completed within 200–400 ms with no detectible intermediates. The Ti, Zr and Hf systems involved a liquid phase with a typical combustion front velocity of $5\text{--}6 \text{ mm s}^{-1}$. The Nb and Ta systems have no liquid phase with a combustion front velocity of $1\text{--}2 \text{ mm s}^{-1}$, and are truly *solid* combustion systems. This study provides a new avenue to chemical dynamics and macrokinetics of high-temperature solid-state reactions.

Joe Wong, E.M. Larson, P. A. Waide and R. Frahm

SPECIAL REPORT

Portugal, past and present

The early days



Crystallography was taught in the early thirties as an independent discipline at the Geology Departments, Faculty of Sciences of Porto and Lisbon Universities. The didactic book “Cristalografia” published in 1942 by Domingos Rosas da Silva from Porto was a reference and teaching tool for decades. In 1980, “Elementos de Cristalografia” by Frederico Sodré Borges (also from Porto) expanded the topics covered by the previous book, introducing chapters on X-ray Crystallography and physical properties of crystals.

The first applications of X-ray crystallography appeared in Coimbra in 1923, as part of the PhD thesis of José Custódio de Moraes.

In 1930, a brilliant graduate student of the Physics Department, João R. de Almeida Santos, was awarded a research grant to work at the Physics Laboratory of Manchester University, UK, on X-ray determination of crystal structures, under the supervision of Sir Lawrence Bragg. In January 1935 he obtained his PhD with a thesis entitled “The Structure of Anhydrous Cobaltous Chloride, CoCl_2 , at Room and Very Low Temperatures; Cæsium, Rubidium and Thallium Salts of Certain 12-Heteropoly Acids”. On his return to Coimbra, Almeida Santos trained another research student, Luiz Vaz de Sampayo, who then had the opportunity to work at University College in London, from 1951 to 1953, under the supervision of Dame Kathleen Lonsdale. This pioneering work certainly constituted the embryo of the present X-Ray Diffraction Center in Coimbra.

In Lisbon, Professor of Mineralogy Carlos Torres de Assunção developed the identification of minerals by X-ray powder diffraction, and in co-authorship with Julio Garrido from Madrid, the first edition of “Tables pour la détermination des minéraux au moyen des rayons X” was published in 1952 by the Laboratory of Mineralogy and Geology, Lisbon Faculty of Sciences. This mineralogical trend was pursued by a research student, José Lima-de-Faria, under the supervision of Peter Gay at the University of Cambridge, UK. Part of that work was published in 1964 by the Junta de Investigações do Ultramar as volume 112 of the series “Estudos, Ensaio & Documentos”, entitled “Identification of Metamict Minerals by X-ray Powder Photographs” which became one of the most quoted reference works in the metamict minerals field.

In 1964, a small research group in Coimbra led by Luis Alte da Veiga, began investigations of the crystal structures of metals and alloys, in particular those of Cr_3Si and related intermetallic compounds. The

scope of this research grew rapidly, progressing towards interdisciplinary research topics using a variety of X-ray and neutron diffraction techniques.

Since then, many centres have emerged throughout the country in new areas of research. The following chapters in this article describe current research topics, organized by scientific fields.

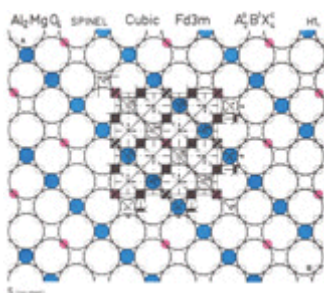
The present

Physics and Crystallography: At the X-ray Diffraction Centre for Materials Research (CEMDRX) (Physics Department, Coimbra University), single crystal X-ray diffraction is used to obtain accurate measurements of electron density distributions in crystalline solids. The results are compared with state of the art *ab-initio* calculations using density functional or LCAO-HF methods [1a]. Synchrotron radiation scattering studies of magnetic and electronic properties of solids are performed by members of CEMDRX at the ESRF in Grenoble. In particular, the novel technique of Resonant X-ray Magnetic Scattering, which combines diffraction and spectroscopy, is used to investigate the magnetic and electronic structure of lanthanide and actinide compounds [1a,].

References

[1a] University of Coimbra, Physics Dept., CEMDRX, Margarida Costa (guida@pollux.fi s.uc.pt), Maria José Almeida (ze@pollux.fis.uc.pt), José António Paixão (jap@pollux.fi s.uc.pt), Ana Matos Beja (ana@pollux.fi s.uc.pt), Manuela Ramos Silva (manuela@pollux.fi s.uc.pt).

[1b] University of Coimbra, Physics Dept., CEMDRX, Lourdes Andrade (lourdes@pollux.fi s.uc.pt)



Top sheet of the condensed model figuring out spinel crystal structure (curtesy of J. Lima-de-Faria).

Mineralogical Crystallography and Crystal Chemistry: Since the establishment of nomenclature for crystal structure types and their classification by José Limade-Faria and Maria Ondina Figueiredo in the Seventies, Crystal Chemistry has been developed at the Crystallography and Mineralogy Centre (CCM) of the Tropical Research Institute (IICT) in Lisbon along two lines.

A successful 2D+1D way of representing closest-packed structural arrangements (condensed models) of crystal structures invented by J. Lima-de-Faria in the sixties was extended to the analysis of loose atomic packings, complex intermetallics and silicates (pyroxenes, amphiboles, micas and feldspars), thereby encompassing an extensive domain of thousands of structures. In parallel, new software was developed for automatic plotting of such condensed crystal structure representations.

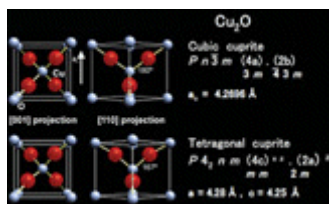
The elucidation of structural relationships between minerals and their structural classification, culminating in 1994 with the publication of “Structural Mineralogy; an Introduction”, was followed by a series of three volumes on the structural classification of minerals (J. Lima-de-Faria, Kluwer Academic Publishers, 2001-2004).

Recently, these structural insights are being used to develop models for innovative applications, reviewing nanomineralogy from a crystallographic perspective^[1].

The identification of copper minerals used to produce color variation in ancient glasses and glazes illustrates the powers of spectroscopic techniques based on the absorption of either soft or hard X-rays at synchrotron facilities.

References

[1] CCM-IICT - Crystallography and Mineralogy Centre, Tropical Scientific Research Institute, Maria Ondina Figueiredo (mof@fct.unl.pt), Teresa Pereira da Silva (teresa.pena@ineti.pt).



Crystallography and XANES spectra simulation: idealized tetragonal structure of Cu_2O allowing non-linear Cu-O-Cu bonds as expected in a glass. (M.O. Figueiredo, J.P. Mirão, *Applied Physics A* (2006) 83, 499-502).

Materials science: Symmetry theory, mathematical crystallography and advanced experimental techniques for structural analysis are being combined by researchers at CCM in Lisbon^[1] to study less ordered systems. Researchers from the Geophysics Centre of Évora University^[2] and CENIMAT (Materials Science Centre, Universidade Nova de Lisboa)^[3] are collaborating in the study of the electronic structure of solids.

The Lisbon group is also examining the crystal chemistry of natural nanophases found in regoliths from semi-arid regions, terrestrial analogues of Martian red soils and synthetic dispersed metal nanoclusters in glasses.

In the Physics Department of Aveiro University [4], the epitaxial growth of crystalline thin films on commercial crystalline structures is analyzed by physical vapour deposition (PVD) and sputtering techniques. Thin films of epitaxial manganite prepared by laser ablation on several oxide substrates are studied by triple axis XRD to determine lattice parameters, misfit and orientation tilting. Crystallographic studies are complemented by real space techniques and emission channelling using radioactive isotopes. XRD analysis of light emitting epitaxial heterostructures includes symmetric and asymmetric reciprocal space mapping, in-plane diffraction and X-ray reflectometry.

The focus of residual stress analysis of textures in the Physics Department of Coimbra University^[5] is: (i) improvement of experimental techniques for residual stress evaluation, enabling their use in new engineering applications; (ii) analysis of industrial techniques used in manufacturing, control and optimisation of processes; and (iii) modelling and numerical simulation of residual stresses.

At the European synchrotron facility, investigators from CENIMAT, New University of Lisbon^[3], are using X-ray microtomography to study particle distribution in SiC particle-reinforced functionally graded aluminium composites and Ni-Ti shape memory alloys (SMA).

References

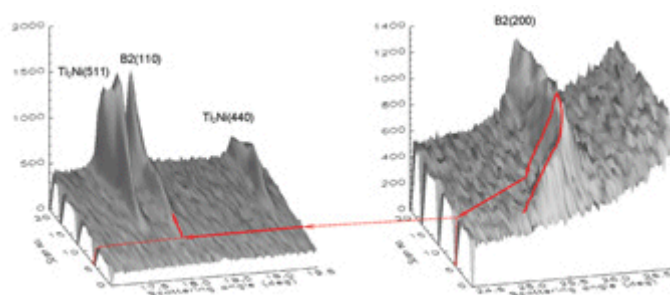
[1] CCM-IICT - Crystallography and Mineralogy Centre, Tropical Scientific Research Institute, Maria Ondina Figueiredo (mof@fct.unl.pt), Teresa Pereira da Silva (teresa.pena@ineti.pt).

[2] Évora University, CGE – Geophysics Centre, José Mirão (jmirao@uevora.pt).

[3] New University of Lisbon, Faculty of Sciences and Technology, CENIMAT – Materials Research Centre, Maria Ondina Figueiredo (mof@fct.unl.pt), Francisco Braz Fernandes (fbf@fct.unl.pt), João Pedro Veiga (jpv@fct.unl.pt).

[4] University of Aveiro, CICECO – Research Centre in Ceramic Materials and Composites, João Rocha (rocha@dq.ua.pt).

[5] University of Coimbra, Physics Dept., CEMDRX, António Morão Dias (morao.dias@dem.uc.pt), António Castanhola Batista (castanhola@ci.uc.pt), José Carlos Prata Pina (zepina@ci.uc.pt) João Paulo Nobre (joão.nobre@dem.uc.pt).



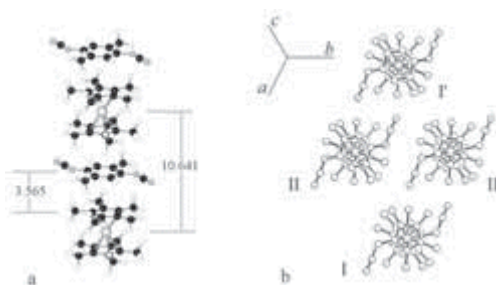
In-situ study of the sputter deposition of NiTi SMA thin films at the ROBL beamline (ESRF). Real-time structural design during magnetron deposition is illustrated (N. Schell, R. Martins, F. Braz Fernandes, *Applied Physics A: Materials Science & Processing* (2005) 81, 1441-1445).

Neutron diffraction: A neutron reactor has been dedicated to physics research in Portugal since the early fifties and neutron diffraction instrumentation at the facility will soon be available to the crystallographic community as well.

However, members of the CEMDRX (Coimbra University) have been already been using European neutron facilities for at least two decades to conduct single crystal neutron diffraction studies of electron density in magnetic materials such as lanthanide and actinide intermetallics^[1,2], oxides^[1] and heavy-fermion^[1-2] compounds. Elastic and inelastic scattering techniques are used to obtain information on static and dynamic properties. Such studies have more recently been extended and/or complemented using synchrotron radiation).

References

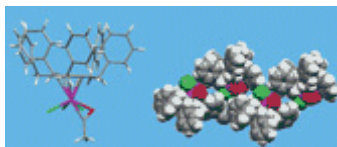
- [1] University of Coimbra, Physics Dept., CEMDRX, Margarida Costa (guida@pollux.fis.uc.pt), Maria José Almeida (ze@pollux.fis.uc.pt), José António Paixão (jap@pollux.fis.uc.pt), Lourdes Andrade (lourdes@pollux.fis.uc.pt), Ana Matos Beja (ana@pollux.fis.uc.pt), Manuela Ramos Silva (manuela@pollux.fis.uc.pt).
- [2] Instituto Tecnológico e Nuclear, Chemistry Dept., António Pereira Gonçalves (apg@itn.pt), Manuel Almeida (malmeida@itn.pt), Laura Pereira (lpereira@itn.pt), João Carlos Waerenborgh (jcarlos@itn.pt)



Review on molecular magnets based metallocenium and bis-(dichalcogenate) metalates, "Metallocenium Salts of Radical Anion Bis-(dichalcogenate) Metalates" (V. Gama, M.T. Duarte, *Magnetism: Molecules to Materials V*, Joel S. Miller and Marc Drillon (eds), Wiley-VCH, Weinheim, (2005) p 1-40).

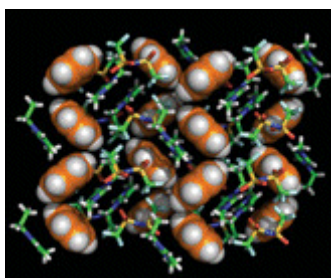
Small molecule crystallography: Maria Arménia Carrondo initiated X-ray diffraction studies on organometallic and coordination compounds in Lisbon in 1979. The first automatic four-circle diffractometer was installed in Coimbra in 1981 while Lisbon got its first one in 1986 at ITN (Instituto Tecnológico e Nuclear). A rotating anode arrived at IST (Instituto Superior Técnico) in 1990 and the first CCD was installed at IST in December, 2005. Shared use of these instruments by the two Institutions has led to the solution of 120 structures per year as part of research projects on synthetic organic, inorganic and organometallic chemistry, catalysis, materials and ionic liquids. In Lisbon at Centro de Química Estrutural (CQE-IST)^[1], and at the Chemistry Department of ITN^[2], molecular and crystal structure determination focus on structure-property and structure-activity/reactivity relationships of organic semi-conductors, a wide range of organic and planar coordination based molecules, and molecular magnets. New X-ray studies, structural databases and theoretical calculations are combined to determine

structure-activity relationships in compounds exhibiting high hyperpolarizabilities, homogeneous catalysts for the polymerization of α -olefins and vanadium compounds having insulin-enhancing and anticancer activities. Other areas of investigation include pharmacophores, polymorphism using co-crystallizations and characterization of ionic liquids.



Molybdenum and Tungsten Cyclopentadienyl Oxo Monomers and Dimers: Syntheses and Applications in Olefin Epoxidation Catalysis (A.M. Martins, C.C. Romão, M. Abrantes, M.C. Azevedo, J. Cui, A.R. Dias, M.T. Duarte, M.A. Lemos, T. Lourenço, R. Poli, *Organometallics* (2005) **24**, 2582-2589).

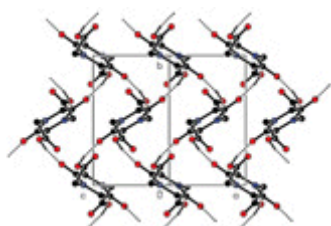
At ITQB (Instituto de Tecnologia Química e Biológica) [3] crystal structure determination focus on organic compounds with chiral properties, new organometallic complexes and the structural characterization of ionic liquid compounds synthesised at ITQB.



Crystal structure of an intercalated ionic liquid, data collected at ESRF synchrotron (ID29 beam line).

Condensed phase behaviour of ionic liquid - benzene mixtures: Congruent melting of a [emim] [NTf₂]•C₆H₆ inclusion crystal (J. Lachwa, I. Bento, M.T. Duarte, J. N. C. Lopes and L. P.N. Rebelo, *Chem. Commun.* (2006) 2445-2447)

At IBMC (Instituto de Biologia Molecular e Celular) and ICBAS (Instituto de Ciências Biomédicas de Abel Salazar) [4] xanthone derivatives, triterpenes and diterpenoids with medicinal use are being extracted from plants and marine sponges and characterized. The coordination around the metallic center of copper and nickel complexes is being correlated with dissociation enthalpies.



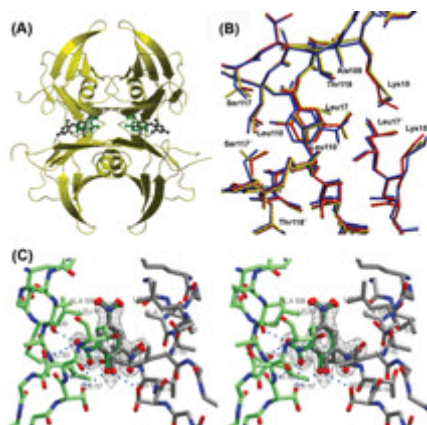
R_4^4 (30) rectangular rings in 2,5-dioxo-piperazine-1,4-diacetic acid. The crystal structure of 2,5-dioxo-piperazine-1,4-diacetic acid was determined showing the formation of a network of rectangular R_4^4 (30) rings consisting of four neighbouring molecules joined by strong hydrogen bonds. (M. Ramos Silva, A. Matos Beja, J. A. Paixão, A.J.F.N. Sobral, L.M.L. Cabral, A. M. D'A. Rocha Gonçalves *Acta Cryst.* (2003) **C59**, 562-563)

At CICECO (Research Centre for Ceramics and Composites, Chemistry Department of Aveiro University) [5] synthesis and molecular design of new macrocyclic receptors for the selective binding of organic substrates and toxic metals is being guided by molecular mechanics, molecular dynamics and quantum mechanical calculations.

In Coimbra, at CEMDRX, targets for structural studies include aminoacetic acids and their N-methylated derivatives having unusual electric properties [6,7], chiral compounds and catalysts [6], molecular rotors exhibiting ferroelastic behaviour [6], Langmuir-Blodgett films related to kinetic reactions in biological membranes, molecular electronics and optical data storage [6], five-membered heterocyclic compounds with potential anti-tumor and anti-leukemic activity and steroidal anticancer drugs [6].

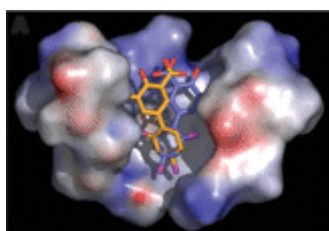
References

- [1] Technical University of Lisbon, Instituto Superior Técnico, Centro de Química Estrutural, M. Teresa Duarte (teresa.duarte@ist.utl.pt), M. Fátima M. Piedade (mdpiedade@fc.ul.pt), João Ferreira da Silva (joao.luis@ist.utl.pt), Adelino L. M. Galvão (adelino@ist.utl.pt), M. João Ferreira (mjoao.ferreira@netcabo.pt). [2] Instituto Tecnológico e Nuclear, Sacavém, Dept. de Química, Isabel C. Santos (icsantos@itn.pt), Dulce Belo (dbelo@itn.pt), Sandra Rabaça (sandrar@itn.pt). [3] New University of Lisbon, ITQB – Instituto de Tecnologia Química e Biológica, Isabel Bento (bento@itqb.unl.pt), Pedro M. Matias (matias@itqb.unl.pt). [4] University of Porto, IBMC - Instituto de Biologia Molecular e Celular and ICBAS - Instituto de Ciências Biomédicas de Abel Salazar, Ana M. Damas (amdamas@ibmc.up.pt) and Luis Gales (lgales@ibmc.up.pt). [5] University of Aveiro, Dept. de Química, Vítor Félix, (vfelix@dq.ua.pt). [6] University of Coimbra, Physics Dept., CEMDRX, Margarida Costa (guida@pollux.fis.uc.pt), Maria José Almeida (ze@pollux.fis.uc.pt), José António Paixão (jap@pollux.fis.uc.pt), Lourdes Andrade (lourdes@pollux.fis.uc.pt), Ana Matos Beja (ana@pollux.fis.uc.pt), Manuela Ramos Silva (manuela@pollux.fis.uc.pt). [7] University of Minho, Physics Dept., Etelvina Matos Gomes (emg@fisica.uminho.pt).



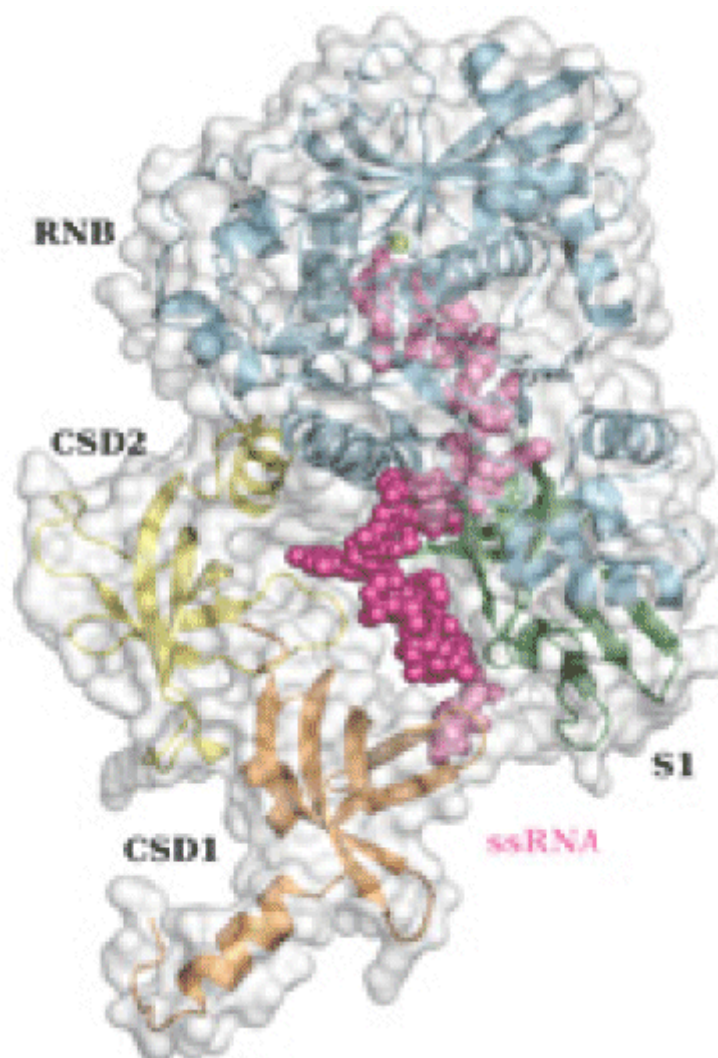
The binding of 2,4-dinitrophenol to wild-type and amyloidogenic transthyretin. (a) Localization of DNP (green) in the TTR hormone-binding channel. The thyroxine (grey) binding site is also shown. (b) Superposition of the DNP-binding site in the different human TTR variants. TTR-WT-DNP is depicted in yellow, TTR Y78F-DNP in red and TTR L55P-DNP in blue. (c) Detailed stereoview of the interactions established between DNP and WT-TTR. (E. Morais-de-Sa, R.M. Neto-Silva, P.J. Pereira, M.J. Saraiva and A.M. Damas *Acta Cryst* (2006) **D62**, 512-519) (PDBIDs 2B14, 2B15 and 2B16).

Protein crystallography: At ICBAS and IBMC [1] the molecular mechanisms underlying amyloidosis of transthyretin (TTR) is being studied. The current focus is on human transthyretin variants and transthyretin amyloid fibrils and the design of amyloid inhibitors and disrupters, on fasciolin, a small antigen secreted by the parasite *Fasciola hepatica*, and on other proteins including enolase, glutamine synthetase, biliverdin reductase and thrombin.



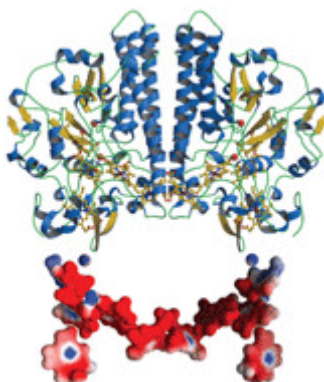
Human transthyretin in complex with iododiflunisal: structural features associated with a potent amyloid inhibitor. The electrostatic surface representation of the AA'-binding site is presented along the x-axis. The two symmetry equivalent positions of the ligands are shown in orange and blue. (L. Gales, S. Macedo-Ribeiro, G. Arsequell, G. Valencia, M.J. Saraiva and A.M. Damas, *Biochem. J.* (2005) **388**, 615-621). (PDBID 1Y1D)

The Macromolecular Crystallography Laboratory at ITQB (Instituto de Tecnologia Química e Biológica) [2] has contributed to the understanding of 3D-structures of metalloproteins involved in electron transfer processes, including multiheme cytochromes, iron-sulfur and iron storage proteins. Recent projects involve structural studies of proteins related to cell adhesion during inflammatory processes in humans, a ribonuclease involved with the degradation of mRNAs, a lactase required for the assembly of the *Bacillus subtilis* endospore coat, complexes of β -cinnamomin, an elicitor from a phytopathogenic fungus, a fish osteocalcin, and some enzymes involved in the synthesis of polysaccharides.



Unravelling the dynamics of RNA degradation by RNase II and its RNA- bound complex - Cartoon of RNase II – RNA complex showing domains CSD1 (orange), CSD2 (yellow), RNB (light-cyan) and S1 (green), the Mg ion as a sphere (green) and RNA in spheres (pink) (C. Frazão, C.E. McVey, M. Amblar, A. Barbas, C. Vonrhein, C.M. Arraiano and M.A. Carrondo, *Nature* (2006), **443**, 110-4.

Collaborations with the Schering AG Berlin pharmaceutical company have supported the study of the androgen receptor ligand binding domain and a double mutant of this receptor in complex with a synthetic agonist. The structural characterization of catechol -O- methyltransferase with novel inhibitors that have potential use in Parkinson's Disease therapy has been studied in collaboration with the Portuguese pharmaceutical company BIAL.



The crystal structure of the cytochrome c nitrite reductase (NrfA) from *Desulfovibrio desulfuricans* ATCC 27774. The heme arrangement is shown and the calcium sites are evidenced as large spheres. Below is represented the electrostatic potential mapped at the heme surfaces. (C.A. Cunha, S. Macieira, J.M. Dias, G. Almeida, L.L. Gonçalves, C. Costa, J. Lampreia, R. Huber, J.J.G. Moura, I. Moura, M.J. Romão *J. Biol. Chem.* (2003), **278**, 17455-17465.

Many Biochemistry/Biology groups at ITQB are working with certain pharmacologically important protein membranes and the crystallography group has recently begun efforts to crystallize them.

The Protein Crystallography group at REQUIMTE (REde de QUÍmica e TECnologia), Universidade Nova de Lisboa (UNL) ^[3], studies metalloproteins and proteins involved in electron-transfer processes. Targets include molybdopterin enzymes, xanthine oxidase-related enzymes, nitrate reductases and formate dehydrogenases, cytochrome c peroxidases, a membrane-bound multi-heme nitrite reductase, a sixteen-heme cytochrome, non-heme Fe/S proteins (e.g., superoxide reductase, a protein responsible for the scavenging of superoxide radicals in the cell), and several components of the “cellulosome”, a supramolecular assembly present in microorganisms that efficiently convert cellulose and its monomers to ethanol. Initial results include the first structures of the type I cohesin-dockerin complex and of several carbohydrate-binding modules (CBM). Also seen on the cover - protein published in *Structure*, **10**, 1261-1272 (2002).

References

- [1] University of Porto, IBMC - Instituto de Biologia Molecular e Celular and ICBAS - Instituto de Ciências Biomédicas de Abel Salazar, Ana M. Damas (amdamas@ibmc.up.pt) and Luis Gales (lgales@ibmc.up.pt), Pedro J. B. Pereira (ppereira@ibmc.up.pt).
- [2] New University of Lisbon, ITQB – Instituto de Tecnologia Química e Biológica, M. Arménia Carrondo (carrondo@itqb.unl.pt), Pedro M. Matias (matias@itqb.unl.pt), Carlos Frazão (frazao@itqb.unl.pt), Margarida Archer (archer@itqb.unl.pt), Peter F. Lindley (lindley@itqb.unl.pt), Isabel Bento (bento@itqb.unl.pt), Francisco Enguita (fenguita@itqb.unl.pt), Maria Luísa Rodrigues (mariar@itqb.unl.pt), Colin McVey (mcveyo@itqb.unl.pt), Daniele di Sanctis (sanctis@itqb.unl.pt), Meike Stelter (meike@itqb.unl.pt), Célia Romão (cmromao@itqb.unl.pt), Tiago Bandejas (tiagob@itqb.unl.pt).
- [3] New University of Lisbon, Faculdade de Ciências e Tecnologia, REQUIMTE/CQFB, Maria João Romão (mromao@dq.fct.unl.pt), Ana Luisa Carvalho (alcarvalho@dq.fct.unl.pt), José Trincão (trincao@dq.fct.unl.pt), Shabir Najmudin (shabir@dq.fct.unl.pt).



Participants at the NATO Advanced Study Institute in Algarve, 1987

Teaching: Crystallography was originally taught as an independent discipline in the Geology Departments of Porto and Lisbon Universities. However, since the fifties, it has been taught along with

Mineralogy and Solid State Physics and Chemistry in most Portuguese universities. Two decades ago Crystallography began to be taught at Universidade Nova de Lisboa as an independent and basic discipline within a course on Materials Science and Engineering along with Crystal Chemistry under the guidance of Maria Ondina Figueiredo.



Participants at the NATO Advanced Study Institute at Vimeiro, 1987.

Courses, meetings and conferences: During the past 25 years, ten international conferences covering a broad range of crystallographic topics, including synchrotron, X-ray, and neutron radiation, XAFS, SEXAFS techniques and their application to electron density studies and materials research, and biological and medical science have been organized and conducted in Portugal, including NATO Advanced Study Institutes, a Sagamore conference and the 1997 European Crystallographic Meeting (ECM 17).



Participants at the Summer School in Luso, 1998.

The first BioCrys-Course on 'Fundamentals of Modern Methods in Biocrystallography' at the Instituto de Tecnologia Química e Biológica in Oeiras, in October, 2002, was organized by Maria Arménia Carrondo and Thomas Schneider. The course covered fundamental theoretical concepts of macromolecular crystallography and was geared toward scientists in the early stage of their crystallographic career. This is particularly important due to the rapid development of the field and the fact that many young researchers no longer receive any formal education in crystallography.



Participants at the BioCrys course in Oeiras, 2004.

A second and third edition of this course took place at ITQB, Oeiras, in November 2004 and October, 2006.



Maria Ondina Figueiredo and George Jeffrey in a poster session at ECM 17 in 1997.

Involvement with European Crystallography Meetings (ECMs): Portugal has been involved with the organization of several ECMs by participating in the Programme Committee of ECM 16 (Sweden), ECM 18 (Czech Republic), and ECM 19 (France).



An overview of the Conference Dinner of ECM 17 at the Electricity Museum.

However the most significant contribution to crystallography was the organization of ECM 17, which took place in Lisbon in 1997. This was a joint effort involving the entire senior Portuguese crystallographic community along with many students. Maria-Ondina Figueiredo chaired the Scientific Committee and Maria Arménia Carrondo chaired the Organizing Committee. This meeting hosted over 900 participants from 47 different countries. The scientific programme included 3 plenary lectures, 12 session lectures, 36 mycosymposia on macromolecules; small and medium sized molecules; minerals, materials, inorganic compounds; techniques and instrumentation; and multidisciplinary studies.

A satellite meeting on 'Validation and refinement of macromolecular structures' took place just after the ECM 17. It was organized by Ana M. Damas at IBMC-Porto and over 100 participants from 17 different countries attended the meeting.



The Organizing Committee and the President of ECC at the opening ceremony of ECM 17 in Lisbon, 1997.

Involvement with the European Crystallographic Committee (ECC), European Crystallographic Association (ECA) and the IUCr: José Lima de Faria represented Portugal on the ECC since its founding in 1973. When the ECA was created during ECM17 in Lisbon, Maria Arménia Carrondo became an Officer of the Executive Committee. Maria Teresa Duarte was elected ECA treasurer in 2000 at ECM19 and still holds this position. Presently Ana Margarida Damas and Margarida Archer are the Portuguese representatives on the ECA Council.



A group of Crystallographers at the Conference Dinner at ECM 17 in Lisbon, 1997.

IUCr involvement also started with José Lima de Faria as the Portuguese representative to the General Assembly until 1996 when he was followed by Maria Arménia Carrondo who was elected in 1999 to the IUCr Executive Committee (August 1999 - August 2005). Since 1999, Margarida Costa, Ana Margarida Damas and Maria Teresa Duarte have represented Portugal at the IUCr General Assemblies. Maria Arménia Carrondo was designated Chair of the IUCr Sub- Commission on the Union calendar (August 2002-August 2005). She was a member of the European Crystallographic Association Committee for the

Max-Perutz Prize in 2006.

Membership in the European Synchrotron Radiation Facility (ESRF): In 2004 the ESRF in Grenoble celebrated its 10th year of user operation. Although not among one of the twelve European contracting countries, Portugal was the first to join as an Associate Member in 1998. Portuguese scientists have used the ESRF for projects in the areas of protein crystallography, chemistry, physics, and materials and environmental sciences. Portuguese scientists have been involved in the ESRF Council and in the Scientific Advisory Committee as well as sitting on Evaluation Panels for projects in these research fields.

Portugal became an Associate Member of the Partnership for Structural Biology (PSB) just after it was founded in November 2002. The Partnership's goal is to make use of the structural biology expertise and techniques available at the Grenoble site to build an integrated resource for structural genomics and proteomics in Europe that will focus on proteins with medical interest. ESRF, the European Molecular Biology Laboratory (EMBL), the Institut Laue-Langevin (ILL) and the Institute of Structural Biology (IBS) were the local founding members of the PSB. A number of pharmaceutical companies have also joined the PSB as Associate Members.

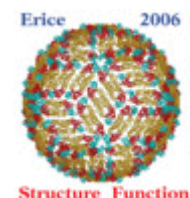
Maria Ondina Figueiredo, Margarida Costa, Ana Margarida Damas, Maria Teresa Duarte, Maria Arménia Carrondo

MEETING REPORT

38th course: structure and function of large molecular assemblies

38th course: structure and function of large molecular assemblies

Erice, Italy, June 8-18, 2006



The major focus of the meeting was on structure and related function for several families of biological macromolecules, with some prominence being given to viruses. The topics covered included structural investigations of small molecule interactions with proteins, multiprotein cellular assemblies, viruses and their interactions with host-cell receptors and antibodies and entire cells. A fantastic array of new protein structures solved using experimental techniques including crystallography, electron microscopy, nuclear magnetic resonance and single-molecule spectroscopic techniques were presented. State-of-the-art advances in technology were highlighted, and the limitations and challenges of the individual approaches were discussed.

Notwithstanding the enormous variety of biological systems described and investigated, a number of common themes emerged. Major advances have often been the result of close interactions among structural biologists using diverse techniques and biologists, chemists, and physicists—multidisciplinary collaborations that can lead to great synergy. The “molecular machines” analogy linking the functioning of large multi-component assemblies with macroscopic machines was frequently invoked and the importance of understanding integration of the components was constantly emphasized. Beautiful computer graphics—both still and animated—of molecular and cellular processes were prevalent and left meeting participants with many vivid images of our expanding molecular atlas of living organisms.

Very exciting progress has occurred since the first Erice Meeting on Macromolecular Crystallography in 1976 when the community was small, although the meeting organizer, Michael Rossmann, claimed “We are already too many!” At that time efforts were focused on studies of proteins with great natural abundance, a few tRNAs, and several plant viruses. Three-dimensional electron micrographic reconstruction techniques were in their infancy. In the intervening 30 years, numerous advances have revolutionized the field of structural biology at all levels. Recombinant DNA technology has made it possible to clone and overexpress even naturally scarce gene products in sufficient amounts for structural investigation, and improvements in microbiological and biochemical technology have permitted scale-up for production of high quality samples for many purposes. The size of structures that can be determined has expanded by orders of magnitude, thanks to technological advances such as synchrotron radiation, high speed computers, superconducting magnets, and algorithmic developments in crystallography.

Another striking feature of the meeting was how our understanding of biology and biochemistry is constantly being related to explanations on the molecular level. Nowhere was this more apparent than with macromolecular structure and the role of conformational changes in regulating and promoting biological processes. Molecules are able to recognize each other through basic chemical interactions, but dramatic changes in molecular shapes can occur as a result of environmental factors such as pH, ionic strength, and the presence of other molecules including co-factors such as ATP, a common unit of energy currency in biology. A number of systems were described in which binding of ATP and other factors led to

large conformational changes and how subsequent chemical processing such as hydrolysis of ATP can lead to regeneration of the original resting conformation. An interesting insight from these collective presentations was that the largest conformational changes are often seen to occur upon binding of a co-factor such as ATP; the energy of hydrolysis is harnessed to bias directionality, and ensure time's arrow, rather than to cause the largest movements. Most lectures and photos can be found at <http://www.crystallrice.org/erice2006/2006.htm> by clicking respectively on the pointers "The Virtual Course" and "Pictures by Eddy Arnold".

Howard Einspahr presented a copy of *International Tables Volume F: Crystallography of Biological Macromolecules*, as the IUCr Journals Prize to Bert Janssen (NL) for the best poster presented by a young scientist.

There were 149 scientific participants from 28 countries : eleven participants that were also at the very first Erice meeting on Crystallography of Molecular Biology received a mug with reproductions of the logo of the meeting. Amongst them, obviously, Michael Rossmann who in addition was presented with a unique ceramic plate celebrating his return as scientific Director of the event – an unexpectedly heavy workload - after 30 years.

The anonymous questionnaire filled in by participants resulted in traditional figure of merit of 3.30 (highest possible was 4) compared with a 3.25 in 2005. The average figure obtained from the question "How do you score the value of the meeting to you - from 0 to 100" was 88.8, just a bit lower than the record value 90.5 obtained in 2005.

Eddy Arnold and Lodovico Riva di Sanseverino



MEETING REPORT

ICDD powder diffraction workshop

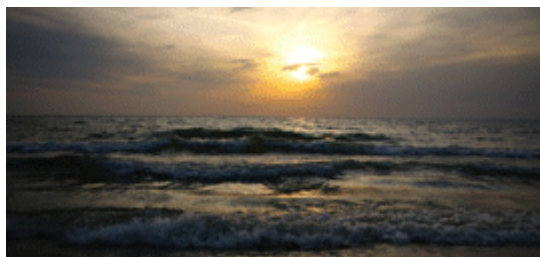
Novosibirsk, Russia, October 18-20, 2005

Evgeny Antipov

A Powder Diffraction workshop was held to present an overview of the ICDD activities, introduce the new version of the PDF-4 database; discuss applications of powder diffraction techniques; and to introduce researchers and students to the "Grant-in-aid" program of the ICDD. The workshop was organized by the Research and Education Center of Novosibirsk State U., the Boreskov Inst. of Catalysis and the Inst. of Solid State Chemistry and Mechanochemistry of the Siberian Branch of the Russian Academy of Sciences and conducted by the ICDD. Representatives of the ICDD (J. Faber, E. Antipov and R. Shpanchenko) delivered many of the lectures to the 66 registered participants from institutes in Novosibirsk, Krasnoyarsk, Ulan-Ude, Omsk, Tomsk, Barnaul, Tyumen', Kemerovo, Novokuznetsk, and Irkutsk. Nine young participants from outside Novosibirsk were supported by the Civilian Research and Development Foundation (CRDF, USA).



The plenary lectures covering various aspects of powder diffraction: techniques for getting high-quality high-precision powder diffraction data, the use of the facilities of the Siberian Synchrotron Radiation Centre (A. Shmakov, A. Ancharov, and M. Sharafutdinov), high-pressure structural studies of molecular crystals, polymorphism of drugs and biomimetics (E. Boldyreva), variable-pressure and variable-temperature studies of zeolites (Yu. Seretkin), application of the cation sublattice method in inorganic crystal chemistry (S. Gromilov), studies of nanomaterials and nanosystems (S. Tsybulya), electron density analysis of short- and long-range ordering in amorphous and disperse materials (E. Moroz). Poster topics ranged from the "Fine details of the structure of MCM-41" (S. Kirik), "*In situ* X-ray powder diffraction and catalysis" (L. Plyasova), to "X-ray diffraction studies of ancient pottery" and "X-ray powder diffraction studies of pharmaceuticals" (T. Drebuschak, and E. Boldyreva). A special session was devoted to the details of preparing data for a submission to the PDF.



The participants had time to discuss research experiences and consult with the experts from the ICDD. Each participant received a package of ICDD informational materials, copies of the lectures, and working and demo-versions of computer programs. Novosibirsk is one of the leading research centers in the field of X-ray powder diffraction in Russia and is recognized internationally for *in situ* structural studies under extreme and variable conditions, structural studies of nanocrystalline materials and techniques in synchrotron radiation diffraction studies.

Elena Boldyreva and S. Tsybulya, Co-chairs of the Local Organizing Committee

MEETING REPORT

School on biological crystallization

Granada, Spain, May 22-26, 2006



An International School on Biological Crystallization (ISBC) was held in Granada, Spain in May, 2006 under the auspices of the IUCr Commission on Crystal Growth. The school was for postgraduate/postdoctoral students and research scientists from industry and academia and focused on the crystallization of biological materials. The 119 participants came from 24 different countries on five continents.



Lectures and practical demonstrations were presented by 22 experts in the field of crystallization of biological macromolecules, drugs and bioactive compounds, polymorphic precipitation, and biomineralization. (The full program is available at <http://isbcgranada.org>.) The first day of the School dealt with the fundamentals of crystallization from solution. Introductory lectures included an overview of the history of protein crystallization, lectures on the physicochemical properties of solutions, nucleation and crystal growth theories and mass transport processes, and included a video of *in situ* crystal growth. The students and participants heard vivid and lively lectures covering all aspects of protein crystal growth, including high-throughput, additives, post-translational modifications, and new crystallization strategies. A highlight was the performance of the ISBC “ensemble” (Alex McPherson, Madeleine Ries, Terese Bergfors and Juan Manuel Garcia-Ruiz) in a hands-on demonstration of batch, vapor diffusion, dialysis or counterdiffusion experiments. After a busy day we walked to the Alhambra for a romantic night tour of the Arabian Nazaríes Palace.



Practical training during ISBC was organized in an innovative and lively format we called a Demonstration Fair. During one whole day, 15 specialists presented 5-20 minute practical sessions. Participants organized their own learning program “*a la carte*” from the experiments on polymorphism,

chocolate crystallization, membrane protein crystallization, seeding of crystals, robotics, and light scattering techniques. The Demonstration Fair is an excellent teaching tool because it provides the students with an opportunity to interact personally with the teacher, to watch at finger distance how to perform the experiments, to do them themselves, to plan their teaching schedule on the fly, to devote more time and attention to some particular demonstration and -if necessary- to attend some a second time. The Demonstration Fair is very demanding and was only possible thanks to a team from the Laboratorio de Estudios Cristalograficos led by José Gavira, Fermin Otálora and Luis Gonzalez-Ramirez. Our experience in designing a “space experiment” at Cape Cañaveral or Baikonur made it possible to install and remove the lab benches on the hotel premises in a few hours.



Another initiative tested in ISBC was to merge the communities of protein crystallization, small molecule crystallization and biomineralization. We ran the risk of phase separation or “demixing” of the two communities. However, to the surprise of many of us, this did not happen. The cross-interaction was very intense and, in the opinion of students and teachers, it was a major achievement of the ISBC. The fourth day started with protein crystallization on an industrial scale and then we moved to polymorphism and high-throughput screening of pharmaceutical compounds, crystallization of lipids and computational methods, and ended with two good tasting talks on ice cream and chocolate crystallization. At night we visited the gypsy district of Sacromonte for a *tapas* dinner in the cave of *Venta del Gallo*, followed by a Flamenco Fiesta and a return to the hotel along the river Darro and the Alhambra.



The last day featured talks on crystallization databases, a crucial tool for understanding crystallization, biomineralization and biomimetic materials. Models for the formation of biominerals were reviewed as well as tools for studying textural characterization. Then followed talks on the precipitation in living organisms of calcium carbonates, oxalates and phosphates, the mineralization process of eggshell formation, production of materials inspired by biomineral structures and self-assembly of hierarchical mineral structures. Six prizes were offered by the IUCr (*International Tables* Volumes A, B and F) and Triana Science & Technology (GCBs and Crystallization mushrooms) to the best posters. Student teams from Italy, Japan, Spain, France, Chile and Belgium were honored by an international panel chaired by Howard Einspahr. We have produced a CD containing all the lectures and demonstrations performed during the School including posters and pictures provided by the participants.

Juan Manuel Garcia-Ruiz

OBITUARY

Bela Ribar (1930-2006)

Professor Bela Ribar died suddenly on March 22, 2006 in Novi Sad, Serbia. He was born September 5th 1930 in Debeljača, Yugoslavia. He started his academic career at the Faculty of Sciences in Sarajevo in 1958. Being a grantee of the Swiss National Fund, he spent three years at the Crystallography Dept. of Bern U., where he obtained his Ph.D. degree in 1969. He joined the Faculty of Sciences in Novi Sad (1970), became a full professor in 1980. In 1987 he became a member of the Academy of Sciences and Arts of Vojvodina (VANU) and a permanent member of the Serbian Academy of Sciences and Arts (SANU) in 2000. In May 2004, he became a the foreign member of the Hungarian Academy of Sciences (MTA).

He published over 200 papers in the field of crystallography most of them in leading international journals and he made significant scientific contributions by studying the crystal structure of a series of inorganic and organic substances and minerals. According to Science Citation Index (through end of 2001) his results were cited over 1000 times in various scientific publications of different branches of fundamental research.

During 25 years of activity in Novi Sad he did a lot for the development of structural crystallography in the region of Vojvodina. He was the founder and the head of the Laboratory for Crystal Structure Analysis within the Institute of Physics of the Faculty of Sciences until his retirement. He shared his knowledge and experience with great enthusiasm with his collaborators as they prepared their M.Sc. and Ph.D. theses under his supervision and became prominent researchers themselves. He was one of the founders and active members of the Yugoslav Center for Crystallography. He was also the first president of the Serbian Crystallographic Society founded in 1991, which, mostly due to his scientific reputation, soon joined the European Crystallographic Assn and the IUCr (1992/3). He served for many years as a referee for the international journals *Acta Crystallographica* and the *Journal of Solid State Chemistry* and he was a member of the Editorial Board for publications from the Yugoslav Center for Crystallography.

Aleksandar Kremenovic, Vice-President, Serbian Crystallographic Soc.

OBITUARY

Kira Mirsky (1935-2006)



In 1958, after graduating from the Potyomkin Inst. in Moscow, Kira Mirsky joined the Structural Analysis Lab of the then Soviet (now Russian) Academy of Sciences and initiated her career as a solid-state physicist/crystallographer.

She became known to scientists working in the field of the organic solid state through her work with Alexander Kitaigorodsky. Together, they developed a simple, fast, and reliable method for the calculation of lattice energies in organic crystals in a scheme called the atom-atom potential method. She authored or co-authored many of the most significant papers of that era that later appeared in English in *Soviet Physics Crystallography*. Kira's pioneering efforts and careful consideration of the implied issues, both in the physical interpretation and in the parameterization, made possible the success of the method. It is still widely used today in molecular dynamics and Monte Carlo simulations, molecular recognition studies, drug design, and other modeling methods.

Kira was among the many talented scientists who emigrated from the Soviet Union to Israel in the early 1970s. She was quiet and reserved, but with a sparkle and smile that revealed a warm and friendly countenance. She joined the Structural Chemistry Department at the Weizmann Inst. of Science in Rehovot, then headed by Mendel Cohen with whom she developed a sorely needed new force field for chlorine which is still a standard in the field.

In the late 1970s, she collaborated with Joel Bernstein on a study of *trans*-stilbene. The molecule crystallizes in space group P21/c with two crystallographically independent half molecules in the asymmetric unit, and its structure was first reported by J.M Robertson in the 1930s. In an elegant mixed crystal experiment Kitaigorodsky had shown that the two half molecules were energetically inequivalent. Kira and Joel wanted to see if lattice energy calculations could account for this energetic inequivalence. She dove into the problem in her usual quiet and very competent way, said nothing for a couple of months, and then presented Joel with a superb computational study that became their joint publication in *Acta Crystallographica*.

Ken Trueblood had met Kira in 1965 when he was on sabbatical leave in Moscow. They formed the kind of friendship that transcends miles, years, and national boundaries, and when she arrived in Los Angeles in 1979, she joined his group and used atom-atom potentials to help characterize disordered structures, and especially, to describe and quantify models for thermal motion studies.

Kira's mother had taught English in Russia, and Kira spoke excellent English. Her knowledge of literature (think "Winnie the Pooh") was wide. So she brought to her speech and manner the colloquialisms and wit that go with speaking several languages, and the special familiarity with life in English-speaking countries that knowledge of literature brings. She was always lively and upbeat and full of humor and ready with a wink or a smile. She possessed great enthusiasm for her work, for nature, and for people.

Kira moved to Ashland, Oregon and Southern Oregon State College, as it was then known, in 1989 where she joined the physics faculty and taught undergraduate physics courses for six years. Sidney Abrahams appreciated finding a crystallographer of her caliber on campus when he arrived two years later. Kira contributed enthusiastically to a study supported by the NSF on the systematic prediction of new ferroelectrics by analysis of their reported crystal structures. Her insight into the geometry of organic

groups and molecules was deep and strongly reminiscent of Kitaigorodsky's, proving most valuable in the study of the physical properties of such materials.

In 1994, Kira moved to Spokane, Washington where she taught physics at Whitworth College. She and her husband, Mike, moved to Seattle in 1999 for a very active "retirement". Kira was a talented linguist and used her gift as a translator, editor, and medical interpreter. She made life better and happier for many people, and she will be remembered for her intelligence, wisdom, love, and laughter. Her knowledge was more than matched by her quiet, dignified demeanor and wonderful traits, middot as is said in Hebrew.

Joel Bernstein, Angelo Gavezzotti, Emily Maverick, S. C. Abrahams, Mike Mirsky, Reuben Rudman, and Ron Stenkamp

AWARDS AND PRIZES

Musić receives award



Svetozar Musić, Senior scientist with the Ruđer Bošković Institute (Zagreb, Croatia) and a member of the Croatian Crystallographic Association, received the 2005 Annual Award of the Croatian Academy of Science and Arts for his outstanding achievements in materials science and crystallography. His research has focused on investigation of intermetallic oxides by X-Ray diffraction, electron microscopy, FT-IR and Raman spectroscopy.

Stanko Popovic

AWARDS AND PRIZES

FEBS Journal award



Nicole LaRonde-LeBlanc, a postdoctoral fellow in the Macromolecular Crystallography Lab., National Cancer Inst. (Frederick, MD, USA), was awarded the 2005 FEBS Journal Prize for Young Scientists. She was the first author of a paper entitled “Structure and activity of the atypical serine kinase Rio1” (N. LaRonde-LeBlanc, T. Guszczynski, T. Copeland, A. Wlodawer, *FEBS Journal* **272**, 3698-3713, 2005), judged by the editors of the Journal to be “the best published in the journal in 2005 that falls within the rules for our *FEBS Journal* Prize for Young Scientists.” The prize includes a check for 10,000€, as well as an all-expenses-paid travel to the 31st Congress of the Federation of European Biochemical Societies, held in Istanbul, Turkey, in June 2006 where she presented there her work on determining the crystal structure and autophosphorylation sites of Rio1, a novel kinase involved in ribosome biogenesis and cell cycle progression. Rio1 and related kinases may become important new targets for designing anticancer drugs.

Dr. Alexander Wlodawer

AWARDS AND PRIZES

2006 BCA-IG Prize



The 2006 BCA-IG prize was awarded to Paul Fewster (PANalytical). Prof. Fewster is widely acknowledged as one of the leading experts on X-ray diffraction world-wide. He has made major contributions to the development of both the apparatus and the analysis of the results and has used this expertise to contribute to the development of a wide variety of electronic and photonic devices.

AWARDS AND PRIZES

2006 Clifford G. Shull Prize



J.M. Carpenter is the recipient of the 2006 Clifford G. Shull Prize of the Neutron Scattering Society of America "For seminal contributions to the development of neutron sources and instrumentation that have had world-wide impact on neutron scattering across a broad range of scientific disciplines, culminating in the optimized design of the Spallation Neutron Source at Oak Ridge."

The Neutron Scattering Society of America (NSSA) established the Clifford G. Shull Prize in Neutron Science to recognize outstanding research in neutron science and leadership promoting the North American neutron scattering community. The prize is named in honor of Prof. Clifford G. Shull, who received the Nobel Prize in 1994 with Prof. Bertram Brockhouse for seminal developments in the field of neutron science. The establishment of the prize was announced at the inaugural American Conference on Neutron Scattering (ACNS) in 2002.

The prize and \$5000 honorarium was awarded at the 2006 ACNS, St. Charles, IL, June 18-22, 2006 (acns2006.anl.gov/).

AWARDS AND PRIZES

ACA 2007 Awards

Randall receives Wood Award



Lisa Randall, Professor of Theoretical Physics at Harvard U., will receive the Elizabeth A. Wood Award at the 2007 ACA Meeting in Salt Lake City next July. The award was established in 1997 to honor the late Betty Wood, author of *Crystals and Light*, and *Science From Your Airplane Window*. The Wood Award is given to those who excel in bringing science to the attention of a wider audience.

Lisa's book *Warped Passages: Unraveling the Mysteries of the Universe's Hidden Dimensions*, (HarperCollins Publishers, New York, 2005), has received high praise from critics. Tim Folger, editor of *Best American Science and Nature Writing*, says that *Warped Passages* "gives an engaging and remarkably clear account of how the existence of dimensions beyond the familiar three (or four, if you include time) may resolve a host of cosmic quandaries.

ACA RefleXions, No. 2, Summer 2006

Gavezzotti receives Trueblood Award



Angelo Gavezzotti is one of the foremost chemical crystallographers in the world. Over a period of more than thirty years he has deeply influenced the way we think about molecular packing in crystals. He is the author of the UNI force field (with G. Filippini), of several crystallographic computer programs, such as OPEC (Organic Packing Energy Calculations), Zip-Promet (a program for the generation of possible crystal structures) and, most recently, the Semiclassical Density Sum Method (Pixel Method) for estimating intermolecular energies, all highly innovative, widely used and successful. He is an outstanding candidate for the ACA Kenneth N. Trueblood Award, which is to recognize exceptional achievement in computational or chemical crystallography.

ACA RefleXions, No. 1, Spring 2006

Herbstein receives Fankuchen Award



Frank Herbstein's work has illuminated chemical crystallographic perceptions for over half a century and has now culminated in the recent publication of his two-volume encyclopedic work on *Crystalline Molecular Complexes and Compounds*. Herbstein's book will be a guide to the perplexed for many years. His lifetime achievements in research, teaching and scholarship eminently qualify him as a most suitable candidate for this award.

ACA RefleXions, No. 1, Spring 2006