

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 16 · Issue 2

Collected archival edition

Original article text and available illustrations

Contents

Letter from the President

Letter from the President	4
---------------------------	---

Letter to the Editor

Need for elemental analysis	6
Proposal to change Statutes	7

IUCr journals news

An investigation into structural changes due to deuteration	9
The β -2 and β' -2 polymorphs of trans-mono-unsaturated triacylglycerols and related fully saturated triacylglycerols	10
Two scandium-biuret complexes: $[\text{Sc}(\text{C}_2\text{H}_5\text{N}_3\text{O}_2)(\text{H}_2\text{O})_5]\text{Cl}_3 \cdot \text{H}_2\text{O}$ and $[\text{Sc}(\text{C}_2\text{H}_5\text{N}_3\text{O}_2)_4](\text{NO}_3)_3$	11
Charge-density analysis of a protein structure at subatomic resolution: the human aldose reductase case	12
8-Methyl-5-methylene-2-oxotricyclo[5.3.1.1 ^{3,9}]dodecan-endo-8-ol	13
Structure of mouse ADP-ribosylhydrolase 3 (mARH3)	14
Evaluation of the focusing performance of bent Laue crystals using wave-optical theory	15
Migration of mercury from dental amalgam through human teeth	16

Regional news

Polish Crystallographic Association	17
The ECA Executive Committee's 'winter meeting'	18

Meeting report

International Crystal Growth Summer School	20
Croatian-Slovenian meeting	22
Reminiscences from HEC-X	24
15th Bruker-Nonius CCD users group meeting	26
Argentinian Crystallography Association 3rd annual meeting	27
Size-Strain V	28
Frolic-Goats high-pressure single-crystal diffraction workshop	30
School on Mathematical and Theoretical Crystallography	31
Erice International School of Crystallography	33

Obituary

John Stezowski (1942 – 2007)	35
Xavier Solans Huguet (1949 – 2007)	36
Book review	
Avoid Boring People, James D. Watson	37
Harwell: from Romans and Runways to Reactors and Research Renaissance	39
Notice	
Eligio Perucca: serendipity across the Atlantic	41
Groom appointed new executive director of CCDC	44
The role of BIOXHIT Training, Implementation and Dissemination (TID) Centres in the use of highly automated macromolecular crystallography beamlines	45
Awards and prizes	
BCA CCG Poster Prize	43

LETTER FROM THE PRESIDENT

Letter from the President



Yuji Ohashi

Since I was elected President of the IUCr in August 2005, the obligation to write this article by the deadline has been very heavy for me. By the time you read one of my articles in the *IUCr Newsletter*, I have had to write a new article for the next issue. Since English is not my first language it has been very helpful to me to have Michael Dacombe (IUCr Executive Secretary), Judith Flippen-Anderson and William Duax, Editors of the *IUCr Newsletter* proof the articles to be sure that my points come across as I intended. This article is the final one for me, since a new President will be elected in Osaka and will write the column for the next issue.

When I was asked to write these articles three years ago it was my intention to bring you the hot news that was being discussed by the Executive Committee (EC) and the decisions made at the EC meetings. In the first issue of this Newsletter, Vol. 1, No.1 (1993), the President of the IUCr, André Authier, said "The primary goal of the *IUCr Newsletter* is to assert and maintain this unity among crystallographers from all nations and all subdisciplines, by offering them a forum where they can follow the evolution of crystallography and where they can express their opinions". The fifteen years that have passed since that first issue has seen a dramatic increase in both the number of crystallographers and in the diversity of the subdisciplines they study. At the 21st General Assembly and Congress being held at Osaka this August the number of presentations will exceed 2,100, the highest number for any IUCr Congresses to date. Moreover, the formation of a new Commission on Crystallography and Art and in Cultural Heritage will be considered by the General Assembly. As the activities of crystallographers represented by the IUCr continue to grow in a wide variety of research fields, I think it most important that the EC should take the lead in finding ways to support this diverse community. In that respect, this column has become increasingly important because it enables the President to communicate directly with the ever broadening structural community.

When I became President, I had misgivings about the financial state of the IUCr. The most important activity of the IUCr is to continue publishing its eight crystallographic journals. Moreover, we publish eight volumes of *International Tables for Crystallography* and the IUCr/OUP Book Series. No other International Union produces such an extensive list of publications. Recently the impact factors of our journals has been gradually increasing, although I do not think the index is the most important way to judge the importance of a journal. The number of readers of our online journals has grown. *Acta Crystallographica* Section E became an open-access journal in January 2008, but I am pleased to say that, even with a submission fee, the number of manuscripts is nearly at the same level as before. These activities have been supported by a variety of crystallographers. The efforts of the Editor-in-Chief, Gernot Kostorz, and the Chester staff, Peter Strickland and others, and almost 200 Editors and Co-editors of the journals have brought about this great success. Through the success of the journal publishing operations, we are able to support young scientists to attend international crystallographic meetings and we can also support crystallographic schools in developing countries by paying the travel expenses of

distinguished lecturers. For the above support more than USD 150,000 has been used each year. Our investment portfolio has also been successful. The value of our assets has increased during the last three years even though many investment banks and associations have fallen into crisis. This success was brought about by the successful judgment of the Convener, Malcolm Cooper, the General Secretary and Treasurer, Sven Lidin, and the members of the Finance Committee. My initial misgivings have gone but we must remain vigilant.

I have been very happy in these three years to work in cooperation with earnest and capable colleagues and staff. I express my sincere thanks to all the members of the Commissions and to the Chester staff, and to all crystallographers worldwide.

Yuji Ohashi, yohashi@spring8.or.jp

LETTER TO THE EDITOR

Need for elemental analysis

Dear Editor

Lachlan Cranswick's excellent review of the IUCr Teaching Commission Newsletter prompted me to look up the original. This took a bit of finding as the published URL is incomplete, but that's another story. It is Anthony Linden's article on "Crystallographic Data Validation - Ten Years On" that has driven me to put fingers to keyboard.

As an analyst as well as a crystallographer it was immediately obvious to me that had ANY of the compounds discussed by Anthony Linden been subjected to elemental analysis, the misidentification of imine as carbonyl would have been immediately apparent. The nitrogen analysis would have been 6 or 7 % out - in some cases, a third of the total nitrogen expected wasn't nitrogen. CHN analysis can be done on 2 mg of sample - less than 2 cubic millimetres - not very much at all. Proper chemical characterisation of compounds presented for structure determination is essential.

I would hope that papers describing crystal structure determinations will not be accepted for samples which are not adequately characterized chemically. What is "adequately characterized"? That must be decided for each case, jointly by author, editor and referees.

David Beveridge

LETTER TO THE EDITOR

Proposal to change Statutes

Dear Editors:

The U.S. National Committee for Crystallography (USNCCr) has proposed seven changes to the IUCr Statutes and By-Laws. For any/all of the changes to take effect they must be ratified by the General Assembly (GA) at the Osaka Congress. The intent of these proposed changes is to ensure maximum diversity in the membership of the Executive Committee (EC) and to emphasize the role of the GA as the forum at which crystallographers direct the work of the Union. The proposed changes fall into three categories.

The first group concerns the number of candidates which must be nominated for the offices of the EC:

1. By-Law §8.5. The second paragraph would be amended to read: At least two nominees shall be presented to the General Assembly for consideration as candidates for election to one of these offices.
2. By-Law §8.6 The following phrase would be deleted: If there are not more candidates than vacancies, the nominations shall be presented to the General Assembly and the candidates shall be considered as elected.

The deletion in §8.6 articulates the election process in light of the changes proposed in §8.5. The current Statutes and By-Laws make it very clear that the ultimate authority of the Union is the GA. In the past it was common for the EC to nominate only one candidate for an office. While having a single candidate for an office undoubtedly simplifies the election process, we feel that the duties of the delegates to the GA are not merely to endorse the recommendations of the EC. We believe that there is no shortage of qualified crystallographer candidates, and are very gratified that the EC has nominated multiple candidates for the election in Osaka. We see no reason that this should not be the case in future assemblies, and would like to enshrine that notion in the By-Laws.

The second group of changes concerns the composition of the EC:

3. Add to Statute §6.1g: one representative from each of the Regional Associates.

The Regional Associates are defined in Statute §1.2i. Representatives of the Regional Associates may attend the General Assembly (By-Laws 1.4), but have no voting power. The three current Regional Associates – the American, Asian, and European Crystallographic Associations – are becoming more important to crystallographers and to the Union. We believe that this growing importance represents an important evolution in the Union and should be recognized by permanent representation on the EC. The benefits of broader representation on the EC should exceed the relatively minor increased costs. It has been noted that this change will introduce members to the EC who have not been elected by the GA. We view this as a good thing, as these representatives will have been chosen by a much larger electorate than the fewer than 100 delegates to the GA. Additionally, while the practice of crystallography is currently distributed approximately equally across the three Regional Associates the distribution of votes in the GA is not (ACA – 13, ECA – 47, AsCA – 17). Additional representation from Asia and the western hemisphere will help the EC better reflect the current diversity of our science.

4. IUCr Executive Secretary, Mike Dacombe, has pointed out that this change in the composition of the Executive Committee would require a change in Statute §5.10(b) to take account of the fact that the representatives of the Regional Associates are not currently elected by the General Assembly and reads: elect the president, the Vice-President, the General Secretary, the Treasurer, and the six ordinary members of the Union [Statutes 6.1 and 6.3]. We should, of course, have a consistent set of Statutes!

5. Statute §6.4 Insert a paragraph describing how these members would be chosen as the next to last paragraph: The representative of each Regional Associate will be that person elected by his or her respective association membership. They are not eligible for immediate re-election to the same office.

Our intent and assumption is that each of the Regional Associates will determine their own selection process, as what works best for one region may not be best for another. Because the other members of the EC serve from GA to GA, it may be best for each Regional Associate to create a new office, rather than have the President of the Regional Associate serve as the EC representative. The ultimate decision would rest with the Regional Associate and the process could well differ from one region to the next.

6. Statute §6.2 Add a third paragraph: The representatives of the Regional Associates are not considered when determining whether there are two or more Officers from any one County.

The intent of the original “not more than two” restriction is clear, and enhances diversity. We see no reason to change it because additional diversity has been incorporated into the membership of the executive Committee.

The final proposed change is largely symbolic:

7. By-Law §1.4 would be amended to remove the following phrase: but they shall not take part in the discussions, unless specifically invited or permitted to do so by the Chair, and they shall have no voting power.

The current wording of this By-Law could be thought to suggest that the establishment does not wish to hear from anyone who could be construed as an ‘outsider’. Such a view may be in keeping with the parliamentary model of the GA but we view the GA as a structured gathering of the worldwide family of crystallographers at which all are welcome. This change would emphasize the right of any member of our crystallographic family to speak at the General Assembly. It would, of course, fall to the Chair to manage any discussions regardless of their source.

We believe that the proposed changes would make the IUCr even more representative of the growing and increasingly diverse crystallographic community.

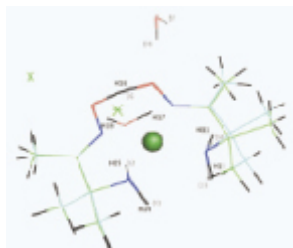
Jim Kaduk, Chair - USNCCr

Katherine Kantardjieff, Vice-Chair-USNCCr

Editors note: Space limitations prevent us from reproducing the full By-Laws and Statutes of the IUCr here. They can be found at www.iucr.org/iucr-top/iucr/statutes.html.

An investigation into structural changes due to deuteration

***Acta Cryst.* (2008). A64, 359–367 [doi:10.1107/S0108767308004807]**



Superimposed bis(3-amino-3-methyl-2-butanone oximate)nickel(II) chloride monohydrate (AM-BONC) structures. Deuterated structure shown in blue and hydrogenated in green.

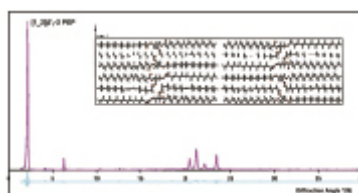
There has been a growth in the experimental determination of the protonation states of proteins. In this study the effect of deuteration on structure was examined by data mining, which yielded 52 small-molecule crystal structures as deuterated and hydrogenated pairs. Differences between these small-molecule structures have been calculated and the results thus far follow the initial assumption. With time, it will become possible to analyse for any differences, at a significant level of precision, of a large cohort of ultra-high-resolution protein structures in H and D forms.

S.J. Fisher and J.R. Helliwell

The β -2 and β' -2 polymorphs of trans-mono-unsaturated triacylglycerols and related fully saturated triacylglycerols

The β -2 and β' -2 polymorphs of trans-mono-unsaturated triacylglycerols and related fully saturated triacylglycerols

Acta Cryst. (2008). B64, 240-248 [doi:10.1107/S0108768108004813]; 249-259 [doi:10.1107/S0108768108004825]



Rietveld refinement result of β_1 -2 PEP (1,3-dipalmitoyl-2-elaidoylglycerol) from high-resolution laboratory data and packing view parallel to the b axis.

With a parallel tempering method (FOX) crystal structures have been solved of the β -2 and β_1 -2 polymorphs of various saturated and trans-mono-unsaturated triacylglycerols (TAGs) using 3 Å resolution synchrotron and laboratory powder diffraction data. Also, the crystal structure has been solved of a novel β' -2 polymorph that melts higher than the β_1 -2. Molecular conformations of symmetric vs asymmetric TAGs in the β_1 -2 polymorph are different while in the β -2 they are the same. The structures imply that a β' -2 to β -2 solid-state conversion is unlikely.

J.B. van Mechelen, R. Peschar and H. Schenk

IUCR JOURNALS NEWS

Two scandium-biuret complexes: [Sc(C₂H₅N₃O₂)-(H₂O)₅]Cl₃·H₂O and [Sc(C₂H₅N₃O₂)₄](NO₃)₃

Two scandium-biuret complexes: [Sc(C₂H₅N₃O₂)-(H₂O)₅]Cl₃·H₂O
and [Sc(C₂H₅N₃O₂)₄](NO₃)₃

Acta Cryst. (2008). C64, m205-m208 [doi:10.1107/
S010827010800824X]



The molecular structure of [Sc(C₃H₅N₂)₄]³⁺.

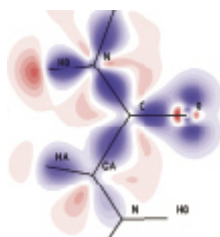
Scandium(III) shows unusual flexibility in its coordination number in complexes, and six-, seven-, eight- and nine-coordinate species are known. When combined with biuret and water molecules, distinctive, near regular, pentagonal bipyramidal [Sc(H₂O)₅(C₃H₅N₂)]³⁺ and square antiprismatic [Sc(C₃H₅N₂)₄]³⁺ geometries arise, suggesting that the counter-ion may play some role in defining the metal coordination preference.

W.T.A. Harrison

IUCR JOURNALS NEWS

Charge-density analysis of a protein structure at subatomic resolution: the human aldose reductase case

***Acta Cryst.* (2008). D64, 567–588 [doi:10.1107/S0907444908006082]**



Deformation of the protein electron density in the peptide bond plane. The blue colour accounts for the accumulation of electron density on the covalent bonds and lone pairs.

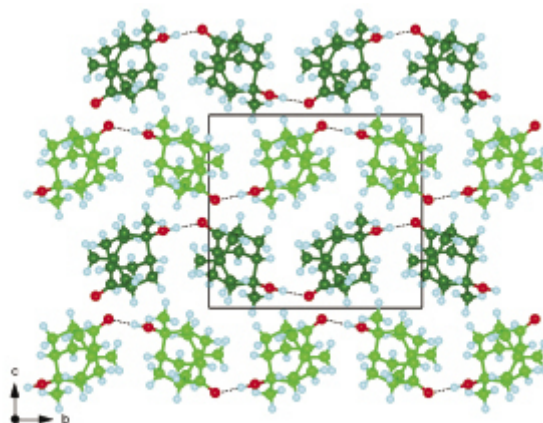
X-ray synchrotron diffraction data are available for human aldose reductase up to 0.66 Å resolution. The protein electron density was refined using a multipolar atom model. Chemically equivalent atoms were constrained to have the same electron density. The refined electron density agrees well with our experimental multipolar atoms database, especially for atoms with many copies in the protein. Upon database transfer, atomic thermal parameters showed a small but systematic decrease. According to the main-chain bond lengths, stereochemical dictionaries may be revised.

B. Guillot, C. Jelsch, A. Podjarny and C. Lecomte

IUCR JOURNALS NEWS

8-Methyl-5-methylene-2-oxotricyclo[5.3.1.13,9]dodecan-endo-8-ol

Acta Cryst. (2008). E64, o841 [doi:10.1107/S1600536808009677]



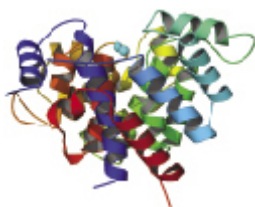
Unit-cell diagram showing the O-H...O=C hydrogen-bonded chain along **b**. Adjacent layers along **c** are chirally pure with alternating chirality. This is indicated by light- and dark-green shading of C atoms. The racemic molecules of this tricyclic compound undergo a considerable degree of enantiomer separation during crystallization. They assemble by means of O-H...O=C hydrogen-bonded interactions into parallel enantiomerically pure chains oriented along the **b** direction, and then further aggregation of these chains results in formation of homochiral layers in the *ab* plane. This type of crystallization outcome, midway between intimate mixing of the enantiomers and conglomerate formation, is a poorly understood phenomenon.

I.Y.H. Chan, R. Bishop, D.C. Craig, M.L. Scudder and W. Yue

IUCR JOURNALS NEWS

Structure of mouse ADP-ribosylhydrolase 3 (mARH3)

***Acta Cryst.* (2008). F64, 156-162 [doi:10.1107/S1744309108001413]**

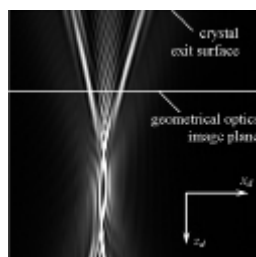


ADP-ribosylation is a reversible posttranslational modification that modulates protein activity in pro- and eukaryotes. The reaction is catalysed by ADP-ribosyltransferases (ARTs) and ADP-ribosylhydrolases (ARHs), respectively. ARTs and ARHs have been divided into a number of subfamilies that are thought to confer substrate specificity. The structure of mouse ADP-ribosylhydrolase 3 has been solved to a resolution of 1.8 Å and is featured as an interactive figure in this publication. Two Mg ions are located in a cleft on the protein surface that pinpoint the active site.

C. Mueller-Dieckmann, S. Kernstock, J. Mueller-Dieckmann, M.S. Weiss and F. Koch-Nolte

Evaluation of the focusing performance of bent Laue crystals using wave-optical theory

J. Appl. Cryst. (2008). **41**, 237–248 [doi:10.1107/S0021889808000617]



Intensity distribution at different distances from a cylindrically bent Laue crystal.

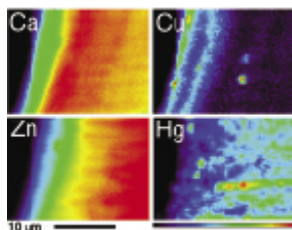
Bent-Laue-crystal optics has proved to be one of the very few optical elements that allows one to focus wide beams of high-energy X-rays (above 30 keV) with high efficiency. The geometrical optics approximation, traditionally used for evaluating the performance of such crystals, has serious limitations on its validity. In our approach, quantitative analysis of the focusing performance of bent Laue crystals is carried out using numerical simulations of the process of propagation of spherical waves through the optical system, based on a rigorous wave-optics treatment, with some significant new findings.

Y.I. Nesterets and S.W. Wilkins

IUCR JOURNALS NEWS

Migration of mercury from dental amalgam through human teeth

J. Synchrotron Rad. (2008). **15**, 123–128 [doi:10.1107/S0909049507061468]



Ingestion of mercury from dental amalgams, with possible negative health effects, has generally been considered to occur directly from filling surfaces. The importance of mercury exposure by direct migration through the tooth was examined by X-ray fluorescence imaging of Hg, Ca, Zn and Cu in human teeth filled with amalgam for more than twenty years. The detection of Hg in areas of the tooth that once contained an active bloodstream and in calculus indicates that both exposure pathways should be considered as significant.

H.H. Harris, S. Vogt, H. Eastgate, D.G. Legnini, B. Hornberger, Z. Cai, B. Lai and P.A. Lay

REGIONAL NEWS

Polish Crystallographic Association

www.chemia.uj.edu.pl/ptk/



The Polish Crystallographic Assn (PCrA) was officially founded in May 2006. The Association office is located at the Faculty of Chemistry, Jagiellonian U. The main mission of the Association is to support development of scientific research in the field of crystallography and the popularization of crystallography and crystallographic methods. The mission is achieved by:

- Organizing seminars, lectures, workshops, etc. to promote crystallography and the use of crystallographic methods by other scientists.
- Organizing courses and summer schools for young scientists and students.
- Collecting and disseminating information about international crystallographic schools and conferences.
- Organizing financial support for young scientists to help them participate in international crystallographic courses, schools and conferences.
- Maintaining contacts with the IUCr, the European Crystallographic Assn and crystallographic associations of other countries.
- Inviting scientists from other countries to visit Polish crystallographic centers, lecture at national and international conferences organized in Poland.
- Promoting research and rewarding achievements in the field of crystallography,
- Other forms of public work.

The first General Assembly of the PCrA was held on June 29, 2006 in Wrocław, at the Inst. of Low Temperature and Structure Research of the Polish Academy of Sciences. Stanisław Hodorowicz (Jagiellonian U., Cracow) was elected the first President. Other members of the Management Committee are: Katarzyna Stadnicka – Secretary (Cracow), Barbara Oleksyn – Treasurer (Cracow), Grzegorz Bujacz (Łódź), Maria Gdaniec (Poznań), Marek Główka (Łódź), Antoni Konitz (Gdańsk), Anna Koziół (Lublin), Zofia Lipkowska (Warszawa), Wojciech Paszkowicz (Warszawa) and Adam Pietraszko (Wrocław).

The PCrA acknowledges three types of membership: ordinary membership (individuals), supporting membership (individuals and corporate bodies), and honorary membership (individuals – outstanding scientists nominated by the Management Committee and accepted by the General Assembly).

Current membership counts 124 ordinary members (including 26 founding members). The Secretary of the PCrA may be contacted at ptk@chemia.uj.edu.pl.

REGIONAL NEWS

The ECA Executive Committee's 'winter meeting'

www.ecanews.org



The Participants of the "Winter Meeting" of the Executive Committee of the European Crystallographic Association held this February in Budapest, Hungary on a pre-dinner 'chance-to-relax' evening walk in the Buda Castle. From left to right: Radomir Kuzel (Treasurer), Petra Bombicz (Secretary), Massimo Nespolo (Webmaster), Hartmut Fuess (Past-President), Abdelmalek Thalal (ECM24 representative), John R. Helliwell (President), Sine Larsen (Vice-President), Luc van Meervelt, Santiago Garcia-Granda and Andreas Roodt (Officers).

Opening the Meeting the President, John R Helliwell, drew attention to the 60th anniversary of IUCr and hearty congratulations and applause were offered. A key matter arising from the ECM24 August 2007 Exec Meeting was the proposal by Yuji Ohashi, IUCr President, to introduce a new category of adherence at the IUCr General Assembly. With the happy endorsement of the ECA Council at ECM24 the identified grouping of countries (ie ECA member but IUCr non-member countries.: Latvia, Turkey, Ukraine, Algeria, Morocco and Tunisia) has now agreed to join the ECA-supported grouping.

A vivid discussion during the meeting on overall ECA strategy was initiated by John Helliwell who stated the four key aspects: 1. Working with the European and African National Societies to 'Add value' but not replace them; 2. Promote continuing professional development of crystallographers via ECMs and training workshops; 3. Foster the study and detailed understanding of crystallography; 4. Diligently provide ECA input to the key European science decision making bodies (e.g. the EC, the ESF, the Innovation for Science in Europe organisation etc) whenever possible. The discussion naturally also assessed the ECA's strengths, weaknesses, opportunities and threats. One threat clearly seen by the Exec Members is the need to increase efforts on the education of the future generations of crystallographers with increased activity needed at all levels. The efforts of the ECA could immediately focus on supporting an initiative within Spain (led by Juan Manuel García-Ruiz and Santiago García-Granda) that could readily lead to the establishment of a European undergraduate/graduate school of crystallography. An education coordinator was identified as being needed and Massimo Nespolo agreed to immediately assume this role to coordinate ECA's efforts and report to the next ECA Council Meeting during the IUCr Congress in Osaka.

A wide variety of Exec Committee 'regular business' also took place and included for example: 1. The funding applications of the organizers of schools, conferences, and workshops to ECA should be supported by a letter from at least one SIG chair; 2. Santiago Garcia-Granda proposed a metrics evidence based system for monitoring the performance of the SIGs that would allow strategically focussed discussions during the Osaka ECA Council Meeting, including any proposed changes in the SIGs; 3. A review of the 2007 ECM24 in Marrakech including final details, registration numbers and the finances that was presented by Abdelmalek Thalal. The successful financial outcome of ECM24 along with the excellent scientific program drew congratulations and applause from the Committee members;

4. The attendance of the ECM25 representative Engin Ozdas with Engin Kendi conferenced in by phone from Istanbul, led to finalised plans for ECM25.

For information on the European Crystallographic Association please visit the ECANews website: www.ecanews.org.

MEETING REPORT

International Crystal Growth Summer School

Park City, Utah, August, 2007

<http://www.crystalgrowth.us/isscg13/index.php>



The 13th International Summer School on Crystal Growth ISSCG-13, was held at the Park City Marriott in Park City, Utah, August 5-11, 2007, hosted by the American Association of Crystal Growth (AACG) under the auspices of the International Organization of Crystal Growth. The School was held prior to the 15th International Conference on Crystal Growth (ICCG-15) in Salt Lake City, Utah.

There were 149 attendees from Armenia, Austria, Brazil, China, Croatia, Czech Republic, France, Germany, India, Israel, Italy, Japan, Mexico, Netherlands, New Zealand, Poland, Romania, Russia, Singapore, Slovak Republic, Taiwan, United Kingdom, Uruguay, and the USA.

Approximately 50% of the attendees were undergrads or post-docs, 20% were lecturers, and the remainder were researchers both new and highly experienced in crystal growth. The large turnout of students from abroad was made possible due to generous sponsorship from the American Chemical Society/Crystal Growth and Design, International Institute of Complex Adaptive Matter (I2CAM), IUCr, Lawrence Livermore National Laboratory, the Olsen Foundation, SAFC Hitech, the US Air Force Office of Scientific Research, and the AACG. About half of the students received some financial support.



A comprehensive series of lectures provided an overview of traditional crystal growth as well as emerging technologies. Lectures encompassed theoretical and experimental aspects of growth, including the thermodynamics, kinetics, fluid dynamics, and growth mechanisms of crystals grown from melts, solutions, and vapors. Lecturers presented *in situ* and *ex situ* characterization of semi-conducting, oxide, metallic, organic, inorganic, and biological crystals, as well as crystal surfaces and interfaces and emergent systems. The technical lectures were complemented by the ISSCG-13 textbook, "Perspectives on Inorganic, Organic, and Biological Crystal Growth: From Fundamentals to Applications," which was published in the AIP Conference Series (Vol. 916, July 2007) and given to each of the attendees.

Questions addressed in the school included: How do surfactants affect crystal growth? What makes an abalone shell so hard? How can nano-particles solve the energy crisis?

Five lectures covering *Crystal Growth Fundamentals* including melt growth with either rough or smooth interfaces (G. Muller, U. Erlangen-Nurnberg), 2-D nucleation and dislocations in solution growth cluster formation (A. Chernov, LLNL), the evolution of vapor growth from HVPE to OMVPE (G. Stringfellow, U.

Utah), defects in crystals (P. Rudolph, IKZ Berlin) and in situ monitoring techniques (K. Ploog, Paul Drude Inst).

Topics in *Simulation and Modeling* included a tutorial on the tools for modeling melt and solution growth processes (J. Derby, U. Minn.), melt flow and crystal growth under applied magnetic fields (K. Kakimoto, Kyushu U.), a mesoscopic model in which the phase field is used to interpolate between macro-experiment and micro-step flow (R. Sekerka, Carnegie Mellon U.), and Kinetic Monte Carlo simulations used to predict the “landscapes” of crystal surface morphology (J. Evans, Iowa State).

The session *Crystal Surfaces and Interface* covered biogenic mineral growth systems (P. Dove, Virginia Tech), kink density and cluster formation in protein crystals (P. Vekilov, U. Houston), the adsorption of impurities on mineral surfaces (S. Parker, Bath U.), surfactant-mediated epitaxial growth (T. Kuech, U. Wisc.) and the structure of the crystal-liquid and crystal-vapor interfaces (E. Vlieg, Nijmegen U.).

Four-lectures on *In situ Characterization* included using optical interferometry to monitor high temperature solution growth in real time (K. Tsukamoto, Tohoku U.), the use of scanning probe microscopy to derive step velocity and free energy at crystal-fluid interfaces (C. Orme, LLNL), VLS nanowire growth using in situ electron microscopy (F. Ross, IBM), and thin film spectroscopic techniques (M. Pristovek, Tech. U. Berlin).

An *Emergent Systems* session addressed biomineralization (L. Addadi, Weizmann Inst.), supramolecular crystal design (M. Lahav, Weizmann Inst.), the impact of impurities on growth steps (J. DeYoreo, LLNL), self epitaxial or templated nucleation that makes abalone shell tougher than steel (X. Yu-Liu, Singapore Natl. U.), nanotubes (G. Galli, UC Davis), and solar energy and nanodot photovoltaics (A. Nozik, NREL).

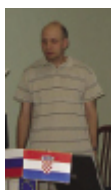
A final series of lectures on *Novel Crystal Technology* addressed bulk and epitaxial SiC growth methods (M. Skowronski, Carnegie Mellon U.), wide bandgap semiconductors fundamental nucleation modes (R. Davis, Carnegie Mellon), properties of nonlinear optical crystals (P. Schunemann, BAE Systems), and novel nanocomposites for artificial bones and teeth (A. Tomsia, LBNL).

The highlight of the banquet at the Canyon’s Red Pine lodge was a biographical lecture by M. McBride (Yale U.) with photographs and notes on “A Portrait of Ostwald’s Life”.

David Bliss

MEETING REPORT

Croatian-Slovenian meeting

Petrcane (Zadar), Croatia, June, 2007

Nenad Tomasic



Radomir Kuzel



Carmelo Giacovazzo



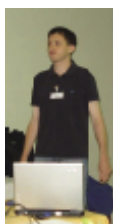
Excursion to Nin, a small town, the capital of the Croatian Kingdom in the 9th century, (inset) the smallest cathedral in the world

The 16th Croatian-Slovenian Crystallographic Meeting was held in Petrcane, a tourist resort on the Croatian Adriatic coast. The meeting was organized by the Croatian Crystallographic Society (SCS), under the auspices of the Croatian Academy of Sciences and Arts (CCA). The Honorary Presidents were Boris Kamenar (CCA) and Ljubo Golic (SCS), and the Co-Chairs were Stanko Popovic (CCA) and Ivan Leban (SCS). There were 85 participants from 13 countries. The meeting was supported by the Ministry of Science, Education and Sport, Pliva, Croatia; Panalytical; Mercator; Bruker-Axs; Rigaku-Molecular Structure Corporation; Zagrebacka Banka, and Hotel Pinija of Petrcane, Croatia. This support is of great

importance, as this meeting was organized without registration fees.



Meeting dinner: Howard Flack with a holy plate in its proper position.



Bojan Kozlevcar

There were four plenary lecturers. Carmelo Giacovazzo (Italy) talked about powerful tools for crystal structure determination and refinement from powder data. Nenad Tomasic (Zagreb) presented work on metamict minerals, – amorphous materials thought originally to be crystalline. Radomir Kuzel (Czech Republic) provided comprehensive insight into the process known as severe plastic deformation. Bojan Kozlevcar (Ljubljana) discussed the correlation between magnetic properties and structures of Cu(II) coordination compounds. The 62 oral presentations covered various fields, from minerals to proteins, from chemical crystallography to structural science, and from computer software to sophisticated equipments.

An excursion to Nin and Zadar included visits to the smallest cathedral in the world (12th century AD), a Roman Forum, and St. Donat Church (dated by 14C spectroscopy to 900 AD).

S. Popovic and I. Leban

Remarkable remarks from the meeting:

There were extraordinary events at this meeting, for example my dear friend P. Segedin used a powerpoint presentation for the first time (I Leban).

Thank you very much for organizing such a successful meeting and for extending extremely warm hospitality to your foreign guests. I was gratified to see the scale and diversity of crystallographic research done in Croatia and Slovenia. (Mariusz Jaskolski, Poznan, Poland).

Thanks very much indeed for the very interesting conference organized in a very professional way, in a delightful place and with very friendly people. (Howard Flack, Geneva, Switzerland).

MEETING REPORT

Reminiscences from HEC-X

Bedlewo, Poland , September, 2007

<http://hec-x.ibch.poznan.pl>



The idea of Heart of Europe Bio-Crystallography (HEC) Meetings that would bring together young protein crystallographers from the center of Europe was conceived in 1998 under the leadership of Rolf Hilgenfeld and Manfred Weiss. Year after year, with growing size and importance, the HEC Meetings have been organized by the participating groups. The 10th Anniversary Meeting, HEC-X, was organized on September 27-29, 2007, in Bedlewo (Poland) by the Center for Biocrystallographic Research of the Polish Academy of Sciences. The Meeting attracted 118 participants, mostly students, from the HEC groups (<http://hec-x.ibch.poznan.pl/>) in Germany, Poland and the Czech Republic, plus 7 commercial exhibitors. In keeping with the HEC tradition, 31 lectures were presented exclusively by young scientists. In addition, there was one HEC lecture given by an invited eminent scientist. The lecturer was Guy Dodson (U. of York, UK) who captivated the audience with a vibrant review of the crystallography, chemistry and biology of insulin.

A committee assembled to select the best HEC presentation included representatives of the HEC Group Leaders, Guy Dodson (Chairman), and Clare Sansom (Birkbeck College, London). The HEC Prize went to Robert Kolodziejczyk (A. Mickiewicz U., Poznan) for his talk entitled "Insect Juvenile Hormone Binding Protein exhibits ancestral fold present in human lipid binding proteins". The Award, *International Tables for Crystallography, Vol. A*, was generously sponsored by the IUCr. Apart from support from the IUCr, we also received a grant from the European Crystallographic Association (ECA), and several donations from commercial sponsors. However, the most generous sponsor was the Polish Network of Cell and Molecular Biology.

The social functions included a barbecue, the HEC Dinner, and an excursion to the Kornik Castle, where the participants had the rare occasion to view the most valuable manuscripts and prints (including a score in Frederic Chopin's handwriting and the first edition of Nicolaus Copernicus' "De revolutionibus orbium coelestium") held in the Library of the Polish Academy of Sciences. There was also a special HEC "History and Reminiscences" session, with lots of memories, anecdotes, laughter, and applause. One of the student participants wrote after the conference "It was my first HEC meeting and now I really understand why everybody likes it so much." This sentence could be the motto of the HEC initiative.



Participants of HEC-X on the stairs of the Bedlewo Castle.

HEC-X was also special because it witnessed the birth of the HEC committee, composed of several of the HEC veterans. One of the tasks of the committee is to designate the next HEC meeting organizer. For the venue of HEC-11, Greifswald has been selected, and the organizer will be Winfried Hinrichs.

Mariusz Jaskolski

MEETING REPORT

15th Bruker-Nonius CCD users group meeting

15th Bruker-Nonius CCD users group meeting

Madison, WI, September 16-18, 2007



George Sheldrick demonstrates the latest release of TWINABS at Bruker-AXS in Madison, WI. Photo by Rob Hooft.

The annual meeting was an opportunity for the users of Bruker-Nonius equipment to discuss the latest advances in the Bruker instrumentation and software development and to share ideas and experiences. The meeting attracted 63 participants from six countries. There were 15 talks during the two morning sessions, four workshops, five poster presentations, and a tour of the Bruker-AXS facility.

The meeting opened with a tour of the chemistry department of the U. of Wisconsin-Madison and a reception dinner by Lake Mendota. The following morning Bruker-AXS experts S. Byram, M. Ruf, E. Hovestreydt and C. Campana presented a detailed overview of their latest instrumentation. After the break M. Olmstead explained how the SHELX command FRAG could be used for refining difficult structural fragments, P. Fanwick and J. Desper spoke about their laboratory practices and the participants toured the Bruker facility. Four workshop sessions led by N. Bhuvanesh, C. Campana (both on powder diffraction), P. Mueller (difficult refinements) and G. Sheldrick (TWINABS) allowed the participants to fine-tune their skills. There were poster presentations from students and a postdoc from Centro de Investigación de Estudios Avanzados (Cinvestav) in Mexico City.

On the second day G. Sheldrick led a discussion of future developments in SHELX, S. Lindeman made a strong case for using CuK α radiation, L. Falvello and B. Foxman spoke about solid state transformations, J. Reibenspies described powder diffraction applications, H. Hope illustrated a cryocrystallography set-up for use in the 5-20 K range, and G. Yap and L. Dahl delivered spirited talks on teaching X-ray crystallography.

The fruitful discussions, availability of experts, and warm atmosphere make user group meeting valuable tools for honing our crystallographic skills. The next meeting will be held in Delft, the Netherlands at the end of September 2008 (contact: Frank van Meurs).

Ilia Guzei

MEETING REPORT

Argentinian Crystallography Association 3rd annual meeting

Argentinian Crystallography Association 3rd annual meeting

San Luis, Argentina, October, 2007



A selected group of participants, during a sightseeing tour at “Potrero de los Funes” lake, some 15 km from San Luis

Over 50 participants submitted 24 contributions (from 82 authors) to the IIIrd Annual Meeting of the Argentinian Crystallography Assn (AACr). There were 14 lectures including four plenary lectures delivered by noted scientists from Argentina and neighboring countries, on the following topics: “Structural Biology at the Pasteur Inst. of Montevideo: a protein crystallography approach in understanding bacterial lipid synthesis regulation” (A. Buschiazzi, Montevideo, Uruguay); “Combined Crystallographic and molecular dynamics study of complexes of calixarene derivatives with contaminant metal atoms”, (O. Piro, La Plata, Argentina); “MGAC (Modified Genetic Algorithm for Crystals and Clusters): prediction of flexible molecules”, (M. Ferraro, Buenos Aires, Argentina); and “Structure and structural transformation of disordered nanomaterials. Experimental and theoretical challenges to structural characterization”, (A. Craievich, Sao Paulo, Brazil).

Contributed papers covered a wide range of disciplines which benefit from crystallography: structural chemistry (organic, inorganic, biological compounds), materials science (crystal growth, phase diagrams, characterization), mineralogy, and, of course, the inescapable “nano” sciences.

The organizers expressed thanks to all the sponsors whose contributions helped ensure the success of the meeting and they plan to organize future meetings on a regular basis.

The IVth Annual Meeting will take place at Bahia Blanca, Argentina, sometime in October 2008 (precise date to be confirmed). For further information please contact baggio@cnea.gov.ar or dlamas@citefa.gov.ar

Ricardo Baggio

MEETING REPORT

Size-Strain V

Garmisch-Partenkirchen, Germany, October, 2007**www.mf.mpg.de/en/abteilungen/mittemeijer/ss-v/welcome.htm**

The 5th Size-Strain conference 'Diffraction Analysis of the Microstructure of Materials' (SS-V) was held October 7-9, 2007 at the Conference Centre Garmisch-Partenkirchen (Germany). The most recent in the series initiated in 1995 in Liptovsky Mikulas (Slovakia) and continued in (Germany), (1998), (Italy) (2001) and the Czech Republic (2004).

The conference dealt with materials microstructure and properties, as they can be studied by diffraction methods, with a special interest in polycrystalline materials. As with the previous Size-Strain conferences, SS-V focused on methodologies for studying lattice defects, residual stress and texture in thin films and surfaces, line-broadening analysis, line-profile fitting and modelling based on fundamental parameters for applications in materials science problems.

The conference was attended by approximately 100 scientists from more than 25 countries including 20 participants from less privileged countries that were supported financially. 36 oral contributions and 50 posters were presented during the three day program put together by a committee chaired by E.J. Mittemeijer and P. Scardi. A small but lively exhibition area hosted booths of sponsoring companies, and in particular the ICDD (see photo below), represented by H. Göbel, D. Rafaja, R.L. Snyder and P. Scardi.



ICDD booth in the exhibition area (from left to right) R. Snyder, P. Scardi and H. Göbel.



The local conference organizers (left to right) A. Leineweber, E.J. Mittemeijer and U. Welzel during the social event at Schloss Linderhof.

New to this years conference were the contributions on atomistic modelling (e.g., H. van Swygenhoven) and several *in-situ* studies of lattice defects and deformation in nanocrystals (I. Robinson, L. Levine, W. Pantleon, O. Thomas, U. Lienert). These research areas are of increasing importance to the size-strain community. A number of interesting contributions described nanocrystalline materials (A. Cervellino, D. Rafaja, S. Billinge). Several reviews and reports dealing with recent advances in many aspects of the study of domain size and lattice defects by the line-broadening method were presented throughout the entire conference (M. Leoni, E.J. Mittemeijer, P. Scardi, R. Kuzel). A further area of large and interdisciplinary interest concerned thin films, (M. Birkholz, R. Guinebretiere, M. Wohlschlögel) and residual stress analysis (Ch. Genzel, P. Withers, T. Gressmann).

The success of SS-V was in a substantial part due to the devoted support by a group of young scientists and students, all members of the department of E.J. Mittemeijer, who assisted the local organizers (E.J. Mittemeijer, A. Leineweber and U. Welzel).

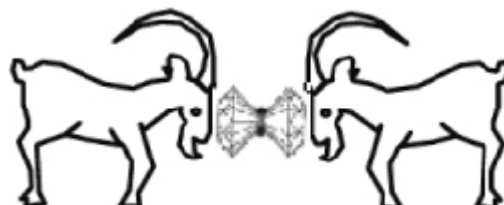
The next Size-Strain conference will be organized in France in 2010. Exact dates and location are soon to be announced by the Chairman, O. Thomas.

E.J. Mittemeijer and P. Scardi

MEETING REPORT

Frolic-Goats high-pressure single-crystal diffraction workshop

Poznan, Poland, April, 2008



Participant of the Frolic-Goats 2008 Workshop (left-to-right): Andrzej Katrusiak, Marek Daszkiewicz, Waldemar Nowicki, Anna Olejniczak, Malgorzata Ratajczak-Sitarz, Marek Szafranski, Katarzyna Jakóbek, Maciej Bujak, Armand Budzianowski, Marcin Podsiadlo, Kamil Dziubek, Roman Gajda, Ulrich Schwarz, Marcin Stachowicz, Maura Malinska, Marcin Jarek, Pawel Piszora, Joanna Loch, Julia Bakowicz, Kinga Ostrowska, Magdalena Mansfeld, Grzegorz Stefanski, Aneta Idczak, Damian Jeczminski, Hanna Piotrowicz. A high-pressure single crystal diffraction workshop was organized in the Faculty of Chemistry, Adam Mickiewicz U in Poznan, April 13-16, 2008. Several research groups in our Faculty share one 4-circle CCD diffractometer, and there is an emphasis on high-pressure measurements. Efficient procedures for preparing the diamond-anvil cell (DAC), loading samples into the DAC, mounting and centering the DAC, increasing the quality of data and precision of results have been developed and were demonstrated at the workshop. Lectures on "Diamond-Anvil Cell (DAC) design, preparation and loading" (A. Olejniczak), "Single-crystal high-pressure diffraction" (A. Budzianowski), "Reduction of DAC high-pressure data" (A. Katrusiak), "Practical aspects of solving and refining high-pressure structures" (M. Bujak, Opole U.) and "Tailoring electronic properties of materials by high pressure" (U. Schwarz - Max Planck Inst., Dresden) were complemented by practical exercises on "DAC preparation, loading and pressure calibration" (R. Gajda) and "X-ray diffraction with a DAC" (A. Budzianowski, M. Podsiadlo). Leisure time was spent sightseeing in Poznan, (capital of Poland between 940-1039, and now the academic centre for 180K students). The Frolic Goats of the renaissance town hall, equipped with the diamond anvils, were chosen as the logo of the Workshop.

MEETING REPORT

School on Mathematical and Theoretical Crystallography

Gargnano, Garda lake, Italy, April/May 2008

www.crystallography.fr/mathcryst/



The IUCr Commission on Mathematical and Theoretical Crystallography, in cooperation with the Commission on Crystallographic Teaching, organized a Summer School on Mathematical and Theoretical Crystallography that was held at Palazzo Feltrinelli, a historical palace on the lake that is currently owned by the U. of Milan.

The School was attended by 40 registered participants from 13 countries and presented 10 lectures by six invited speakers: Mois I. Aroyo (Bilbao), Michele Catti, Milan and Angelo Gavezzotti (Milan), Ulrich Müller, Marburg; Massimo Nespolo, Nancy; Bernd Souvignier (Nijmegen), which covered basic and advanced topics, from fundamental crystallographic group theory to applications in phase transitions, derivative structures, solid-state thermodynamics and molecular packing. Each lecture was accompanied by a series of guided exercises. Didactic material is available for download from the school website.

Most participants were lodged at or near the venue. This allowed for extra evening sessions, during which further exercises and discussions were held.

The abstracts of the posters presented by participants can be accessed on the school website (www.crystallography.fr/mathcryst/gargnano2008.htm).

Young participants got financial support to partly cover their travel and lodging expenses. Eleven grants were assigned from IUCr funds, 8 from ECA funds and 4 from AIC (Italian Crystallographic Assn) funds. The financial aid from Panalytical, from the "Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali" and from the Department of Materials Science of the University Milano-Bicocca allowed the organisers (Angiolina Comotti and Massimo Nespolo) to cover the organisation costs.

Further MaThCryst activities are available at mathcryst.commission@lcm3b.uhp-nancy.fr

Massimo Nespolo, chairman

MEETING REPORT

Erice International School of Crystallography

Erice (Sicily) Italy, May/June, 2008



As the fortieth consecutive Erice course it certainly deserved the RUBY status it was accorded. The drug discovery focus is a recurring theme begun in 1983 and this year's scientific program, the collaboration of directors Colin Groom (UCB UK), and Joel Sussman (Weizmann Inst.), featured several presenters who were regulars from some of the earliest meetings, notably Tom Blundell (U. of Cambridge and Astex Therapeutics) himself now director of the Erice International School of Crystallography, Peter Goodford (U. of Oxford) the creator of GRID, and Trevor Petcher, (University of Bern). The program offered a rich diet of recent structural and bio-informatics results from academia such as Bill Weis' (Stanford) beta-adrenergic receptor and Gabriele Cruciani's (Perugia) probing of the impact of structure on metabolic studies, and examples of drug-design applications from industry including Giovanna Scapin's (Merck) on dipeptidyl peptidase-4 inhibition and Sandra Cowan-Jacob's (Novartis) on countering Gleevec resistance. Piquing widespread interest was the introduction of some nifty new tools for communication of structure by Eran Hodis and Joel Sussman, including *Proteopedia* (www.proteopedia.org/).



Prizewinners and Organizers: (L to R) Taiana de Oliveira, Alice Clark (striking the “di Milo” pose), Joel Sussman, Paola Spadon, Colin Groom and Lodovico Riva di Sanseverino (Ida Rosnes unavailable). In the final analysis, though, the Erice meeting is a school and the emphasis was firmly on students. They made up the majority of the 165 scientific participants and came from countries all across the globe including Turkey, Croatia, Latvia, Lithuania, Brazil, Nigeria, South Africa, India, Malaysia, Australia, New Zealand and Vietnam. After lectures in the morning, the program most days shifted to workshops in the afternoon. These offered demonstration sessions by experts on crystallization, database resources like CCDC, EBI and PDB, CCP4 and computational and bio-informatics tools like CCP4, DOCK and GRID. Among the several innovations targeting young scientists were the award of special priority for younger questioners in discussion periods after lectures and the spirited oral poster sessions where presenters had two minutes to preview and promote their posters. This is a powerful and intense experience for young scientists, one they benefit from greatly in terms of new knowledge, new techniques, new friendships, new self-confidence and new spirit. It was a wonderful thing to witness. Most meals were informal collections around tables at local restaurants and were covered by the registration fees. Many evening meals after workshops were social events: pizza and pasta parties, the

RUBY dinner and dance. In addition there were two excursions to archeological and historical sites of Phoenician and Greek heritage.

None of this could have happened without the careful preparation and precise execution of the schedule by the local organizers, Paola Spadon (U. di Padova), and Lodovico Riva di Sanseverino (U. di Bologna). The computational and communications resources were the work of John Irwin (UCSF), a permanent member of the team. As in the past, an enthusiastic cadre of young scientists, immediately recognizable by their orange scarves, provided all manner of assistance to the organizers.

The Vaciago Award to the young scientist judged most energetic questioner in discussion after lectures went to Brazilian Taiana de Oliveira (PhD student at the U. of Tromsø, Norway). The IUCr presented two poster prizes, a copy of *International Tables, Volume F*, signed by Editors Michael Rossmann and Eddy Arnold, both of whom presented this year, and a copy of *International Tables, Volume A*. They went to Alice Clark (Massey U., New Zealand) for her poster on Filamin A and Ida Rosnes (National University Hospital, Oslo, Norway) for her poster on Endonuclease V (5), respectively.

At the end of the RUBY dance, “RUBY” necklaces and crystals, as well as local souvenir tiles, were awarded to several participants for exceptional displays of elegance, ability, spirit and luck.

Two weeks after the close of the school this year, a better than 75% response to an anonymous web-based questionnaire gave a record average score of 91.41 to the question “Score the meeting 0 to 100, 100 maximum”.

Howard Einspahr

OBITUARY

John Stezowski (1942 - 2007)



Many were saddened by the report of John Stezowski's death on Friday, November 30, 2007. John was a fine crystallographer, a good person and a dear friend.

I met John when he attended a Direct Methods meeting held in Buffalo, NY in 1971. He was a champion of international crystallography and we attended many workshops together in Poland and Hungary in the 1980's where we both made great and lasting friendships. John's enthusiasm for science extended to leaping over the celebratory bonfire breaking his leg at one very memorable meeting in Poland. John moved from the US to Stuttgart, Germany where he taught crystallography, developed a program of analysis of the cyclodextrin structures and mentored many fine students. With assistance from Judy Flippen-Anderson and me he established the IUCr Commission of Small Molecules (now called Commission on Chemical Crystallography). When the Chinese delegation's bid to host the 1990 IUCr Congress lost to the French bid in Hamburg, John approached the Chinese delegation led by Y.C. Tang and proposed that we arrange a special IUCr symposium on small molecule crystallography in Beijing in 1986. At John's invitation Dorothy Hodgkin, Bill Lipscomb, Herb Hauptman and Jack Dunitz agreed to present plenary lectures at the conference, which was a great success.

John returned to the US to establish a crystallographic program at the U. of Nebraska where he once again attracted and trained many excellent students. In Nebraska John continued his elegant studies of the cyclodextrin complexes using crystallography, spectroscopy and molecular modeling to clarify the complex interactions of the disordered guest molecules in these challenging and commercially useful complexes.

William. L. Duax

OBITUARY

Xavier Solans Huguet (1949 - 2007)



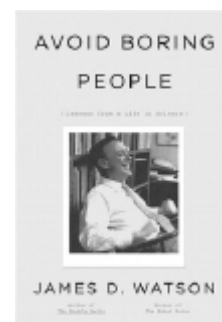
Xavier Solans died suddenly on September 3, 2007 at his home in Sant Cugat (Barcelona). He was 58 years old, full professor in crystallography, and since 2000 he had been Director of the Dept. of Crystallography and Mineralogy at the U. of Barcelona (UB). Xavier finished his studies in Physics at the UB in 1970 and completed his PhD in 1977 with the thesis “Descomposició del factor global de temperatura en el factor de cada àtom, y aplicació del càlcul de la energia de cohesió en la determinació de estructures cristal·lines” under the supervision of Manuel Font-Altaba. After a short period teaching crystallography at the U. of Oviedo, he returned to the UB and was appointed professor in 1984. His principal interest was using direct methods for the systematic crystal structure determination of inorganic and coordination compounds resulting in the publication of approximately 660 SCI journal articles.

He was a very good teacher much appreciated by his students. Many young scientists encouraged and supervised by Xavier received their Ph.D. and are presently working in different laboratories of Spain. He was always amicable and enthusiastic, a quality enjoyed by attendees at the European Crystallographic meetings. He was the Spanish representative when the European Crystallographic Association was founded and occupied this position until recently. As chairman of the Spanish “Grupo Especializado de Cristalografia” he also contributed decisively to the advance and diffusion of crystallography in Spain. He was one of the founding members of the “Club de Cristal·lògrafs Catalans”. He was involved in the creation and subsequent development of the X-ray Diffraction Laboratory at the General Services of the UB. Thanks to his broad expertise in different aspects of crystallography, he solved many important structural problems in collaboration with scientists in the chemical and pharmaceutical industries. He was recently (2006) elected as a permanent member of the Spanish “Real Academia de Ciencias Exactas, Físicas y Naturales”. His premature death truncates a brilliant career and his vitality and enthusiasm will be missed by the Spanish crystallographic community. He will remain in our memory forever.

M. Arriortua, S. Galí, C. Miravittles, J. F. Piniella and J. Rius

BOOK REVIEW

Avoid Boring People, James D. Watson

ISBN 978-0-375-41284-4, 368 pp. (2007) Oxford University Press

Chapter 1 of James D. Watson's "The Double Helix" (Athenaeum, 1968) famously began "I have never seen Francis Crick in a modest mood". Readers of Watson's recent books might feel that they have rarely known Watson to write in either a modest or a reticent vein. Thus, in "Genes, Girls and Gamow" (A.A. Knopf, 2002), the very detailed and indiscreet day-by-day account of his experiences of Cambridge crystallographic and social life during 1953-56 in England, he implies remarkable recall.

Watson's knack for choosing a punchy title is again demonstrated in his latest book "Avoid Boring People". This is virtually an autobiography, beginning with his childhood and education during the Depression and World War II in Chicago and his early research under Salvador Luria. Successive episodic chapters take his career to Europe and the Cambridge collaboration with Crick (which led to the 1962 Nobel Prize) but dwell little on the 1953-56 period.

Chapters follow on his tenure, 1956-1976, on the faculty at Harvard, overlapping for a time with the directorship of the Cold Spring Harbor Laboratory (CSHL), 1968-1994. The narrative effectively ends around 1976 as Watson leaves Harvard to become full time Director of CSHL.

Titles of some of the 15 chapters include "Manners picked up in graduate school", "Manners deployed for academic zing", and "Manners appropriate for a Nobel Prize". Detractors might suggest that manners are an area in which Watson is not well endowed. Consistent with his impatience with those less talented than himself, or holding different opinions, is the advice "Never offer tenure to practitioners of dying disciplines" in the chapter about biology at Harvard entitled "Manners demanded by academic ineptitude".

Though baptized a Catholic, Watson (born 1928) avoided Mass by accompanying his unreligious father, a socialist-leaning Democrat in US politics, on bird walks. Although this knowledgeable fascination with ornithology continued, Watson attributes his lifelong interest in genetics to reading Schrodinger's "What is life?" at age 17. He graduated early from grammar school and high school at the age of 15, began a scholarship to the U of Chicago at a time when President Robert Hutchins introduced compulsory survey courses embracing physical and social services and the humanities. Teaching involved the great books of western civilization rather than conventional textbooks. Later at Chicago U. he began to concentrate on the physical and biological sciences and received a BS degree in 1947 while only 19 years old.

Watson went to graduate school at Indiana U. where he began studying phage under Luria, who was to become a Nobel Laureate in 1969. With a Merck post-doctoral fellowship, he was able to spend a year in Copenhagen, ostensibly to learn nucleic-acid chemistry but, in the end he returned to phage experiments. Watson now realized that to get at the essence of DNA one needed to learn basic crystallography. While Maurice Wilkins at King's, London, was unreceptive to enquiries, John Kendrew accepted Watson in the new MRC Unit, directed by Max Perutz, within the Cavendish, itself headed by Bragg.

Crystallographers are likely to find greatest interest in the chapters reprising the post-doctoral years from 1951 at Cambridge and on the drafting and revising of “The Double Helix” manuscript in the 1960s. Under the chapter title “Manners needed for important science”, Watson reminds readers that, though Crick at 35 had no PhD, he was the pre-war recipient of the prize for experimental apparatus at University College, London, and had accomplished ingenious and effective war-time work on magnetic-mine countermeasures. He also reflects that Rosalind Franklin would have recognized the double helix first had she interacted better with Wilkins and other scientists and entered the model-building race. Incidentally, Peter Pauling, who arrived at the Cambridge Unit in 1952, doubted whether there was a race. ‘Maurice Wilkins has never raced anyone anywhere!’ Watson also acknowledges the contributions of Raymond Gosling at King's, Bill Cochran in the Cavendish, and Jerry Donohue who was there on sabbatical from Caltech.

The chapter “Manners behind readable books”, recounts the gestation of “The Double Helix” and inevitably involves Franklin and her crucial fibre X-ray photographs. In the new book, she is illustrated serving coffee in her Paris laboratory. The original working title for the book, “Honest Jim”, arose from how Watson was addressed ironically by a King's researcher who resented what he regarded as the improper use of Franklin's data. In the Epilogue added to “The Double Helix”, Watson admits that his impressions of Franklin earlier in the book were wrong and he describes her X-ray work at King's as superb. Drafts of the first chapters were composed in the summers of 1962 and 1963, with the rest written in late 1965 during a sabbatical at Cambridge.

Many of the principal characters were highly critical of the frankness and egocentricity of the manuscript, renamed “Base Pairs”, one of them describing it as vulgar popularization. The masterstroke in achieving publication, by Athenaeum since Harvard Press didn't like fights between scientists, may have been Bragg's. The Foreword which still seems exquisitely composed with a deft allusion to Watson's ‘Pepys-like frankness’ reference to the dilemma about trespassing in another's field, and the challenges of competition or collaboration.

In the Preface to “Avoid Boring People”, Watson notes that, while his unpublished writings will eventually be publicly available in the archives, he wanted to be the first to utilize them. Indeed, his remembered lessons at the end of the double-helix chapter includes the maxim ‘Be the first to tell a good story’. While there is no index and the only career summary is on the flyleaf, Watson includes an extensive collection of 3-4 line thumb-nail sketches of his cast of characters, many now Nobel prize winners or distinguished otherwise.

This memoir is replete with anecdotes. Throughout his career, Watson has come across to many as academically arrogant, ruthlessly gifted, breezily chivalrous, disarmingly candid and untroubled by doubt, but possessing a passionate belief in the ultimate value of genetic research for the human condition. He tells a compelling story of a brilliant scientist, astute enough to ask the right questions, to collaborate with or engage bright people, and to take part, as practitioner or manager, in some of the most significant science of the past half-century. “Avoid Boring People” contains some good advice for scientists on their way up - like always having a patron in case, say, an expected grant application is turned down. Crystallographers who have not read any of Watson's recent books should sample this one first.

Derry W Jones

BOOK REVIEW

Harwell: from Romans and Runways to Reactors and Research Renaissance

N.J. Hance, ISBN 0-09553055-0-0, 336 pp (2006), Enhance Publishing, Oxford



Hundreds of crystallographers from many countries have carried out neutron diffraction experiments at AERE Harwell or more recently at the ISIS spallation source at the Rutherford Appleton Laboratory (RAL), Chilton, England. Other X ray scientists use the Diamond synchrotron X ray source nearby. Set up in 1946, AERE was the British secret Atomic Energy Research Establishment but the laboratory complex was always known as 'Harwell', the name of a village in Oxfordshire.

The facilities were constructed on the site of a former Royal Air Force aerodrome from which Horsa troop carrying gliders were towed at the dawn of the D-Day invasion of Normandy in June 1944. Former aircraft hangers and other RAF buildings housed AERE reactors and laboratories for many years. Historically, the Harwell Chilton plateau lies at the intersection of an old Roman road that is over 2000 years old with two long distance pathways, one of them, the Ridgeway, is over 4000 years old (which gave its name to a hostel accommodating visiting scientists).

Nick Hance, a former member of the instrument staff of the DIDO and PLUTO reactors (which supplied Harwell's steady state neutron beams from the late '50s to the '80s) has compiled a history of the Harwell Chilton site and Harwell, in particular. His book outlines historic events before the 20th century and describes pre World War II and wartime RAF activity. It then chronicles the initial build up to a nuclear research station of worldwide reputation, the subsequent de-emphasis of nuclear research and, in the present century, the transformation to a large international science park. Hance is well qualified for this; in his 46 years on Harwell's staff, he first worked on nuclear accelerators, while his later career was in information, marketing and media relations, coupled with considerable lecturing on diverse aspects of Harwell's history. Thus he has experienced many of the changes in Harwell's culture. I still possess a copy of the user guide, dated 1973, to the Badger (neutron) diffractometer on the DIDO reactor by N.J. Hance.

Scientific distinction of the new government scientific establishment was assured by the appointment of John Cockcroft as the first Director of AERE. While still directing the laboratory at Chalk River in Canada, he had from 1945 been discussing the requirements for a UK nuclear laboratory. Cockcroft's Nobel Prize (with E.T.S. Walton) came in 1952 but in 1932 he was in the same laboratory at Cambridge in which James Chadwick discovered the neutron. Unsurprisingly therefore, Cockcroft encouraged neutron scattering experiments. James Thewlis headed the early "Diffraction Branch"; absorption and extinction were investigated by George Bacon and others, utilizing the low fluxes from the early reactors. Bacon and Pease and Bacon and Curry, while not competing with Alpher, Bethe and Gamow yielded entertaining author combinations!

Later, a neutron scatterer, the charismatic Walter Marshall, became head of theoretical physics and then Deputy Director and Director of AERE (1966-1973). By this time many overseas and UK university scientists were utilising the higher steady state neutron fluxes from holes in the PLUTO and DIDO reactors, as they continue to do from ISIS. However under Marshall's Directorship, scientific services

were increasingly offered to industry as the concentration on nuclear powered research steadily decreased.

By the 1980s, other directors, who included the solid state physicist Graeme Low, had to further reduce staff and encourage vigorous marketing of Harwell's commercial services. Fusion research and reactor physics had already left Harwell. In 1989, AEA Technology was launched as a consultancy and services business and subsequently privatised; from the 1990's an extensive program of decommissioning, decontamination and demolition eventually included the DIDO and PLUTO reactors familiar to neutron scientists. The most prominent and idiosyncratic building on site, the Van de Graaff generator, looking like an enormous cigar lighter, was also demolished.

Contemporary neutron scatterers now utilise ISIS, replete with target station 2; its address is Chilton but it is still on the site of the former airfield. The most prominent building on the Harwell Chilton campus is now the Diamond synchrotron X-ray source. Its appearance has been likened to that of an immense flying saucer, the most expensive single scientific investment in the UK for many years. The Harwell international science and high technology park now contains over 100 companies employing 4000 people. Despite Harwell being one of the biggest of such parks in Europe, its staff (and scientific visitors) can still enjoy a congenial rural and scenic environment. Abingdon, the nearest town and home of many Harwell workers is one of the oldest in Britain, while nearby, in racehorse training country, is the Uffington White Horse, an ancient hill carving admired by many visiting scientists.

Over the years, Harwell has engaged in a variety of scientific activities, embracing non destructive testing, advising on the treatment of chemical emergencies, and computing how a catastrophic subway fire was generated at King's Cross, London, in 1987. Such topics are among many described by Hance.

In 35 self contained chapters, illustrated by 300 historic photographs of buildings, people and equipment, Hance tells entertainingly the fascinating story of Harwell's origins, many of its non crystallographic activities during the second half of the 20th century, and how Harwell has metamorphosed into a multi tenanted 21st century international campus. This book should appeal, not just to those with a nostalgia about reactor neutrons, but to anyone who has enjoyed working at the facilities of Harwell or Chilton.

Derry W Jones

NOTICE

Eligio Perucca: serendipity across the Atlantic



Bart Kahr and Davide Viterbo

In a symposium dedicated to the award of the Fankuchen prize to Frank Herbstein, Bart Kahr (U. of Washington), presented a paper entitled “*Eligio Perucca first observed induced optical activity in 1919*”. Perucca was a physics professor at the Politecnico di Torino, who terrorized many generations of engineering students. I was never his student, but I still have his excellent Physics textbook, full of detailed descriptions and beautiful pictures of now obsolete instruments.

Bart Kahr told us that in a 1919 paper (*Nuovo Cimento*, **1919**, 18, 112-154) Perucca had anticipated the discovery of two important effects: induced optical activity, normally attributed to Pfeiffer (*Chem. Ber.* **1931**), and enantioselective adsorption on chiral crystals normally attributed to Bonner (*Science*, **1974**). With modern instruments Kahr and his colleagues repeated experiments, in which Perucca had measured the rotatory power of chiral NaClO_3 crystals grown in the presence of a racemic mixture of a blue dye. They confirmed his observations and in Kahr’s Seattle lab the terrible Professor Perucca became an unsung hero. Kahr found an article on Perucca by V. De Alfaro (a physics professor in Torino) in which Perucca was described as “un personaggio bizzarro”. He then read in the biography of Primo Levi by M. Anissimov that Perucca had been one of the professors who in 1941 refused to assign a thesis to Primo Levi (another Turinese) because he was Jewish.¹ The hero began to look like a “bizarre fascist”. I could not refrain from intervening and took the microphone. After describing an example of Perucca’s terrible treatment of students, I questioned the report by M. Anissimov because Levi was a chemistry student at the University of Torino, while Perucca was teaching physics at the Politecnico, a completely separate academic institution. I also added that in those times everyone had to show sympathy to the regime.

An immediate friendship with Bart was the best outcome of the episode. Joel Bernstein, who was chairing the session, was also impressed by the event and in his description in “ACA Reflexions” he wrote: “Unbeknownst to Kahr, Davide Viterbo was in the audience..... Even before Kahr completed his lecture, Viterbo requested –permission to relate a few personal accounts, confirming Kahr’s anecdotal tales of Perucca’s classroom tyranny. The question of whether Perucca had first observed induced optical activity is still open to debate, but the lecture, and the atmosphere created by that incident and the day long sharing of academic experiences by the speakers provided a fitting close to a unique day of award symposia honoring two distinguished members of the crystallographic community. It was the stuff memories are made of.”

Back in Torino I contacted Vittorio De Alfaro, Perucca’s assistant Luigi Radicati di Brozolo, Perucca’s nephew Gianni Perucca, and Primo Levi’s sister Anna Maria. They all agreed that Perucca was an anti-fascist and that Anassimov’s biography is unreliable. Renato Portesi, who was Primo Levi workmate for years at SIVA, a varnish factory near Torino told me that once he took a sample to test to the physics department of the Politecnico and when he came back Primo Levi mentioned Perucca and said that he attended some of Perucca’s lectures because he was known to make anti-fascist remarks.

In the “Potassium” account Levi tells how he met “the assistant” (N. Dellaporta), who allowed him into his lab. He wanted an experimental thesis, but Jews were not allowed in the labs and he had to be content with a descriptive dissertation on Walden inversion signed by Prof. Ponzio. Milone was Ponzio’s assistant and later my professor of Physical Chemistry.

In conclusion I only have two certainties: Perucca was not fascist and Anassimov’s biography can not be taken at face value. I enjoyed this historical search and I thank Bart Kahr for stimulating it.

Davide Viterbo

1. Primo Levi is my favorite author because I have at least three affinities with him: I am a chemist, I am Jewish and I was born and still live in Torino.

AWARDS AND PRIZES

BCA CCG Poster Prize



The winner of the Chemical Crystallography Group's 'Best Student Poster' prize, sponsored by the IUCr, at the BCA Annual Spring Meeting (York, UK, April 8-10, 2008) was Helena Shepherd (U. of Durham) for poster CP14: "A Variable Pressure Study of a Stepped Spin Transition in an Iron(II) Dinuclear Complex". Helena received a copy of *International Tables Volume A*.

Richard Cooper

NOTICE

Groom appointed new executive director of CCDC



The Board of Governors of the Cambridge Crystallographic Data Centre (CCDC) is pleased to announce that Colin Groom has been appointed as Executive Director of the CCDC as of October 1, 2008, following the retirement of Frank Allen. He is currently Head of Computer-assisted Drug Discovery and Investigative Chemistry at UCB in Cambridge, UK.



Frank Allen (left) and Colin Groom.

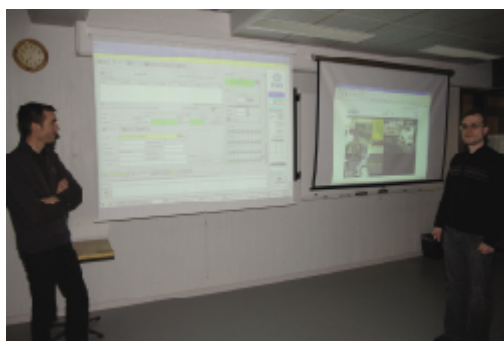
Colin Groom has a BSc in biotechnology and a PhD in protein crystallography from the U. of Leeds, and has held postdoctoral appointments at Leeds and at Massey U., New Zealand. Since then, he has worked in the pharmaceutical industry, joining Pfizer Global Research, Sandwich, UK in 1994, where he established a protein crystallography facility, and then established and led the molecular informatics units in both Sandwich and in the USA. He joined UCB (Celltech) in November 2002. He was Co-director of the International School of Crystallography: *Molecules to Medicines via Crystallography* held in Erice, Italy in May 2008. He has been at the forefront of applying structural information to drug design and has a number of publications and patents in this area. He is a Fellow of the Royal Society of Chemistry, a member of the British Crystallographic Assn, and has contributed to BBSRC and EPSRC activities as a panel member. He is on the Editorial Boards of *Current Computer-Aided Drug Design* and *Current Drug Discovery Technologies*.

NOTICE

The role of BIOXHIT Training, Implementation and Dissemination (TID) Centres in the use of highly automated macromolecular crystallography beamlines



A teaching session at the Poznan TID centre during the 6th Training course, April 7-9, 2008. the participants are being supervised in computer practicals by Santosh Panjikar from EMBL-Hamburg. Biocrystallography (X) on a Highly Integrated Technology Platform for European Structural Genomics (**BIOXHIT**) is an integrated project that has been supported through funds (~10 M €) from the European Union during 2004-2008. All European synchrotron facilities with beamlines for macromolecular crystallography and major software developers are among the 20 partners. The main aim of BIOXHIT, with Victor Lamzin (EMBL-Hamburg) as coordinator, was to develop a pipeline for structural genomics (biology) that will take a protein from the crystallization stage through the data collection at highly automated synchrotron beamlines to structure determination. The evaluators of BIOXHIT from the US and Japan concluded that the project has been very successful in achieving its goals. The next step is to implement remote access that allows users to control experiments being conducted at synchrotrons from home. The project has been successful in implementing European standards for mounting frozen crystals used at the 25 beamlines for macromolecular crystallography that serve about 250 structural biology groups in Europe.



Demonstration of remote access data collection at the ESRF performed as part of the CPP4 workshop held in Oulu, April 21-25, 2008.

It is not trivial to make optimal use of all the new advanced technologies developed in the BIOXHIT project, and it is an obvious challenge to train the structural biology community to become efficient users of the synchrotron beamlines. BIOXHIT has conceived and implemented the concept of special dedicated TID (Training, Implementation and Dissemination) Centres to overcome these difficulties. A special TID committee has looked after these activities. The TID centres were selected based on their scientific excellence, educational experience, experience in use of synchrotron radiation, and links to

other groups in the same geographical area. In 2004 TID centres were established at Oulu University, Finland and at the Inst. of Bioorganic Chemistry, Polish Academy of Sciences in Poznan, Poland. Two additional TID centres were created in ITQB, Oeiras, Portugal and in IMBB-FORTH, Heraklion, Greece. The TID centres have made, and are still making, major valuable contributions to the BIOXHIT project, which comprise developments of the data collection pipeline and training material and, last but not least, to the training of present and future users of the macromolecular crystallography beamlines in Europe. Short accounts of activities at four TID centres follow:

Poznan TID Centre - Mariusz Jaskolski

The Poznan TID Centre used the support from BIOXHIT to organize a modern computer laboratory for training activities and acquire equipment and accessories for crystal handling and shipping and for the implementation of the remote data collection strategy. Two practical workshops on “Structural Biology with Synchrotron Radiation” have been organized every year and thus trained about 150 students. The workshops have been cost-free to graduate and postgraduate students coming from all over Europe and sometimes quite far away (China, Mexico). Leading European (and occasionally American) experts in synchrotron protein crystallography give lectures and teach small-group hands-on practicals, providing the students with exposure to the situation they will face at macromolecular synchrotron beamlines, which includes live data collection sessions at the ESRF. The three day workshop ESRF includes an afternoon get-together (with famous “TID cakes”) and a cultural event. Anonymous surveys of participants’ opinions have been extremely candid and useful. We hope to be able to carry this mission beyond the official timeframe of BIOXHIT.

Oulu TID centre - Rik Wierenga

The first activities of the Oulu TID centre were to become familiar with the most recent data-collection and data-processing protocols used by the BIOXHIT partners. After visits to the ESRF, Grenoble and to the MOSFLM developers at the MRC-LMB, Cambridge in 2005, the first two courses were organized on this theme in 2006. The courses were held in our Linux class room, at the Dept. of Biochemistry, co-sponsored by the Biocenter Oulu. Also in the subsequent two courses, in 2007 and 2008, data collection protocols were included. In 2007, the BUSTER/TNT and SHARP software of Global Phasing Ltd. were presented and remote data collection at the ESRF was demonstrated. In 2008, the course included remote data collection at the ESRF as well as the use of the structure determination pipeline software of the CCP4 package. The last two courses also provided good opportunities for the students to work with their own data. Altogether 84 participants have attended our courses where 24 tutors, mainly from the BIOXHIT partners, have provided a unique forum for in depth discussions with the students. The majority of the participants were from the Nordic and other European countries; altogether the participants originated from 14 different countries, including Israel and India. Our TID activities have also included software (DNA) testing and preparation of manuals and training videos (www.dna.ac.uk/). Another important activity has been our involvement in the remote data collection setup at the ESRF. In this context we have been involved in brainstorming and testing of the e-HTPX and ISPyB database development, which is an integral part of the remote data collection protocol.

Lisbon TID centre - Maria Armenia Carrondo



The participants at work during one of the tutorial sessions at the workshop on "S-SAD diffraction data phasing of macromolecule single crystals from home and Synchrotron X-ray sources" held by the Lisbon TID centre, October 3-6, 2007.

The main activities of the Oeiras TID centre included the organization of training courses and dissemination of the BIOXHIT developments on the use of automation, software advances of ISPyB and DNA and remote data collection at the ESRF. Specific workshops on "S- SAD diffraction data phasing of macromolecule single crystals from home and synchrotron X-ray sources" have been organized, one in 2007 focused on students from Portugal and Spain while the second one in 2008 was directed at students from other European countries. These workshops were attended by 16 students each and speakers were leading scientists in the field from BIOXHIT partners. Students from our TID centre have also participated in other training activities organized within BIOXHIT, namely workshops/courses in Hamburg, Poznan, Oulu and Amsterdam.

Greek TID Centre - Kyriacos Petratos

The Greek TID-Centre for BIOXHIT is a joint effort of the protein crystallographers at the Institute of Molecular Biology and Biotechnology (IMBB) of the Foundation for Research and Technology-Hellas (FORTH) in Heraklion, Crete and the Institute of Organic and Pharmaceutical Chemistry (IOPC) of the National Hellenic Research Foundation (NHRF) in Athens. The centre used BIOXHIT seed-money for several powerful computers that are running up-to-date programs for crystal structure determination and analysis of biological macromolecules. Our Centre has collaborated with the Finnish centre on the preparation of DNA training material. A BIOXHIT supported course on crystallization, data collection and processing was run June 2008 in Heraklion.

The TID centres have played a very important role in training European macromolecular crystallographers. More than 300 European crystallographers have received thorough training at the TID centres making them highly qualified users of the synchrotron beamlines for macromolecular crystallography. The concept of TID centres may also be useful in other projects, resulting in massive amounts of information that can be disseminated to a large scientific community.

The BIOXHIT TID committee

Sine Larsen (chair), Andy Thompson and Paul Tucker