

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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EDITORIAL

In a garden in Cairo

A tale of a crystallographer from Egypt



In 1997, in a beautiful garden overlooking the river Nile in Cairo, I was reading a molecular biology text book. I stared at a magnificent ribbon diagram of insulin and wondered how in the world such atomic details could have been obtained. I could easily imagine the wealth of information retrievable from such a structure and its physiological relevance. At the time, I had a masters degree in medical biophysics with only a shallow knowledge of structural biology. There was not a single structural biology laboratory in all of Egypt. I really wanted to know the power and limitations of NMR and crystallography in determining the three dimensional structures of proteins and DNA. I read several text books but reading was not enough. I wanted to understand the methodology through practice and hands-on experience. I soon realized that I needed a formal education and training in a field that was not available in Egypt. Therefore, I decided to pursue my PhD abroad.

I received a scholarship from Florida State University and joined the Institute of Molecular Biophysics in 1998. One of my rotations was in the crystallography laboratory of Michael Chapman. Looking at the three-dimensional images of the enzyme arginine kinase bound to a transition state analogue was breathtaking. It felt like swimming within a molecule of nanometer diameter. I saw every residue and made measurements at close to atomic resolution. That was so impressive. The power of the technique was immediately obvious to me and I knew then that crystallography was exactly what I wanted to do.

I joined Chapman's group and received my PhD in 2002 with three publications. I am indebted to him for teaching me all aspects of crystallography. He was also instrumental in improving my writing and communication skills.

I finally became a crystallographer! Wow! I had to cross an ocean and complete four years of graduate work to understand that single page I had read in the garden. My mother still wonders why it took me so long to understand one colored figure!

Then I moved to the University of Oregon to work with Brian Matthews who is, by all means, an exceptional scientist and a true gentleman from whom I learnt a lot. He is smart but cheerful, famous yet approachable and serious but very considerate. I spent three years in his laboratory and left with three more papers in my bag. It could not have been better. My family and I immensely enjoyed the magnificent beauty of Oregon (It is a must-visit if you are in the neighborhood).

I am now a faculty member in the Biophysics Department, Cairo University and concurrently work at the structural biology research center of the Photon Factory synchrotron with Soichi Wakatsuki who has provided me with a unique opportunity to develop several structural biology projects while being exposed to beam-line commissioning and operations. I enjoy very much the decent society of Japan and its unique culture.

Recently, I have been going to Egypt more often to teach at Cairo University. Unfortunately, there are still no structural biology laboratories in Egypt (and probably in the entire Arab world!). I get to see very talented students who are passionate and interested in macromolecular crystallography but, regrettably, have no clear path to follow.

In an attempt to change this situation, we have organized a series of workshops and summer schools in macromolecular crystallography at Cairo University. We would also like to establish a state-of-the-art center of excellence for interdisciplinary science in Egypt. The proposed center will encompass modern wet and computational laboratories for macromolecular crystallography linked to the SESAME project. (SESAME – see articles on pages 7-10 – is a synchrotron facility being built in Jordan under the auspices of UNESCO, www.sesame.org.jo). The center is expected to serve scientists from the entire region by providing training and help with the design and execution of experiments. Experiments will be divided into three parts: sample preparation (cloning, protein expression/purification and growing crystals), data collection and computational analysis (data processing, phasing and refinement). Sample preparation and computational analysis will take place in the center with data collection at SESAME.

SESAME is expected to start operations in 2010, however, we prefer not to wait. Partnership and collaborative projects with the international community and synchrotrons around the world could “jump start” this initiative. The IUCr could help coordinate and catalyze these activities. Consortia between SESAME members are also highly encouraged. Our over-arching objective is not only to advance basic science in the region but also to address serious regional problems such as epidemic diseases. Malaria, bilharzias and hepatitis could be targets for structural genomic approaches linked to the international endeavors to combat those diseases.

Funding is being sought nationally and internationally to establish the center. Much like everywhere else, obtaining governmental funds for scientific projects is not easy. Fortunately, the Minister of Higher Education and the administration of the faculty of science at Cairo University have been very supportive. We would certainly appreciate any possible help to support the endeavor.

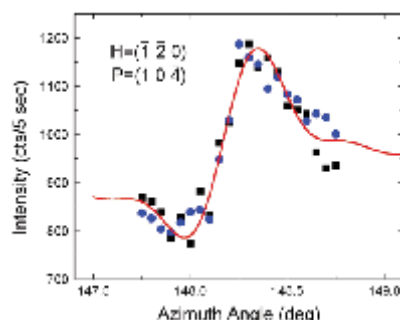
I have a firm belief that education, science and technology have unstoppable power to reform societies and promote mutual understanding and respect. I am optimistic by nature and sincerely hope that ten years from now, when I walk into that same garden in Cairo I will find a number of students engaged in an animated discussion over the latest advances in crystallography!!

Moahmmad S. Yousef, yousef@post.kek.jp

Resonant scattering and multiple Bragg X-ray diffraction in LaMnO_3 ; a classical view

Resonant scattering and multiple Bragg X-ray diffraction in LaMnO_3 ; a classical view

Acta Cryst. (2006). A62, 459-462 [doi:10.1107/S010876730603889X]



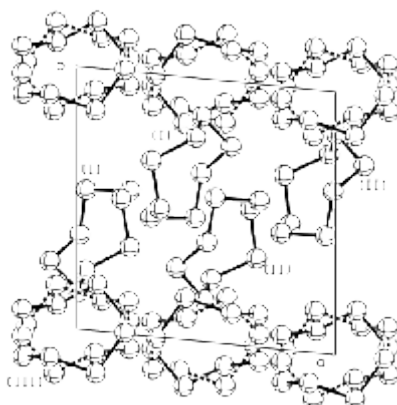
Intensity vs. azimuthal angle for the 10-4 in proximity of full excitation of the -1-20. The 10-4 Bragg reflection is centered at 148.4° . The asymmetry of the profile is clearly visible and is a phase effect, corresponding to a particular model for the charge density.

The mechanism for resonant scattering in LaMnO_3 has been the subject of some controversy between two competing models, leading to different d -electron densities. Forbidden reflections like 300 and 10-4 are turned on by resonance. Three-beam diffraction can be used to resolve ambiguities in determining valence electron densities obtained by means of resonant scattering. The choice between a negative and a positive structure factor is a particular aspect of the phase problem for which the technique of three-beam diffraction is particularly suited.

R. Colella and Q. Shen

Order-disorder transition in monoclinic sulfur: a precise structural study by high-resolution neutron powder diffraction

***Acta Cryst.* (2006). B62, 953-959 [doi:10.1107/S0108768106039309]**



The crystal packing of monoclinic sulfur viewed along the *b* axis, showing the two ordered and one disordered S₈ molecules in the asymmetric unit.

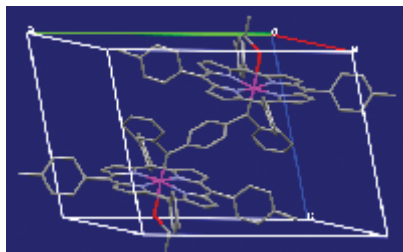
Sulfur is one of the few elements that possess multiple allotropes and associated structural phase transitions. This paper characterizes the order-disorder phase transition in the monoclinic (β form) of octo-sulfur using neutron powder diffraction and also highlights problems encountered as a consequence of the low thermal conductivity of the sample when adopting rapid data collection strategies.

W.I.F. David, R.M. Ibberson, S.F.J. Cox and P.T. Wood

IUCR JOURNALS NEWS

The first metalloporphyrin dimer linked by a bridging phenylenedicarbene ligand

Acta Cryst. (2006). C62, m594-m596 [doi:10.1107/S0108270106043472]



A molecule of the bis[ruthenium(II)-porphyrin]-dicarbene complex in the triclinic unit cell. (Ru: pink, O: red, N: blue, C: gray.)

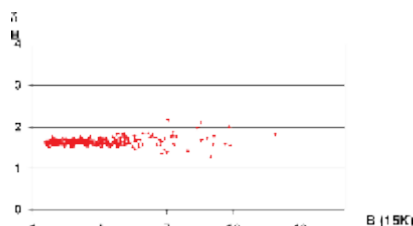
In the first bis[ruthenium(II)-porphyrin]-dicarbene complex, an inversion center is located at the center of the μ -phenylene group, leading to a parallel arrangement for the pair of porphyrin ring systems. The bond lengths and angles compare favourably with literature values for ruthenium-porphyrin-monocarbene complexes. The Ru^{II} ion is displaced out of the C_{20}N_4 porphyrin least-squares plane (by 0.2373 Å) toward the bridging ligand of the C_i -symmetry dimer. The porphyrin ring systems of the dimer thus exhibit mildly domed conformations.

H. Yuge, T.K. Miyamoto, T. Kikuchi and Y. Iwasaki

IUCR JOURNALS NEWS

Ultrahigh-resolution study of protein atomic displacement parameters at cryotemperatures obtained with a helium cryostat

***Acta Cryst.* (2006). D62, 1535-1544 [doi:10.1107/S0907444906041035]**



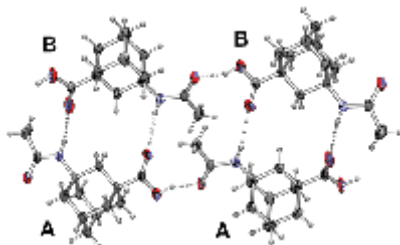
The differences $\delta B = B(60\text{ K}) - B(15\text{ K})$ in isotropic equivalents of ADPs for CA atoms of residues in a single conformation. All values are sorted according to B values at 15 K.

The contribution of temperature and other factors to the atomic displacement parameters (ADP) was estimated by comparison of models of human aldose reductase determined at 0.81 Å resolution and temperatures 15, 60 and 100 K. For ordered atoms, the differences in the isotropic equivalents of ADP were almost constant (about 1.7 Å²) while the character of the changes in ADPs was isotropic as temperature increased from 15 to 60 K. Both decreasing the data redundancy and increasing the resolution cutoff led to an increase in ADPs values.

T. Petrova, S. Ginell, A. Mitschler, I. Hazemann, T. Schneider, A. Cousido, V.Y. Lunin, A. Joachimiak and A. Podjarny

3-Acetamidoadamantane-1-carboxylic acid

***Acta Cryst.* (2006). E62, o5406–o5408 [doi:10.1107/S1600536806045417]**



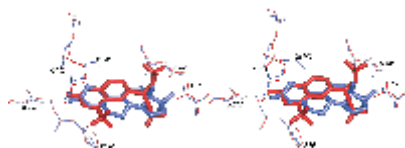
A and *B* molecules of 3-acetamido-1-adamantane-carboxylic acid related by a pseudo-inversion centre. Hydrogen bonds are depicted as dotted lines. The title compound is an intermediate in the preparation of an unnatural amino acid, 3-amino-1-adamantane carboxylic acid. It crystallises in a monoclinic space group with two molecules per asymmetric unit, *A* and *B*, related by a pseudoinversion centre. The intermolecular O–H⋯O hydrogen bonds link the symmetry-related molecules into infinite chains of *A* and *B* molecules parallel to the [101] direction. The intermolecular N–H⋯O hydrogen bonds cross-link these two chains whereas adamantyl cages create a hydrophobic surface around them.

K. Molčanov, B. Kojic-Prodic, N. Basaric and K. Mlinaric-Majerski

IUCR JOURNALS NEWS

Structure of the ligand-binding domain (LBD) of human androgen receptor in complex with a selective modulator LGD2226

***Acta Cryst.* (2006). F62, 1067-1071 [doi:10.1107/S1744309106039340]**



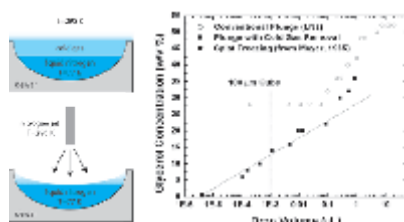
Superposition comparison between the ligands of LGD2226 and R1881 in ligand-AR LBD complexes. Part of the LGD2226-AR LBD complex is shown in red; part of the R1881-AR LBD complex are shown in blue. The androgen receptor (AR) is a ligand-inducible steroid hormone receptor that mediates androgen action, determining male sexual phenotypes and promoting spermatogenesis. LGD2226 is a synthetic non-steroidal ligand and a novel selective AR modulator. Here we reported the crystal structure of the complex of LGD2226 with the androgen receptor ligand-binding domain (AR LBD) at 2.1 Å and compared it with the structure of the AR LBD-R1881 complex. It will aid in further explaining the selectivity of LGD2226 and in developing more selective and effective therapeutic agents.

F. Wang, X. Liu, H. Li, K. Liang, J.N. Miner, M. Hong, E.A. Kallel, A. van Oeveren, L. Zhi and T. Jiang

IUCR JOURNALS NEWS

Hyperquenching for protein cryocrystallography

***J. Appl. Cryst.* (2006). 39, 805-811 [doi:10.1107/S0021889806037484]**



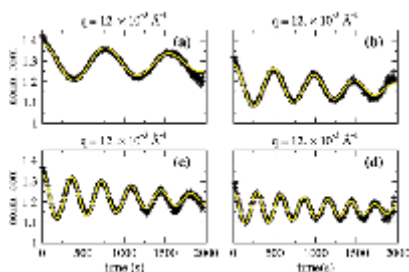
By blowing away the cold gas layer, glycerol concentrations required to achieve vitrification of small sample volumes is dramatically reduced.

When protein crystals are plunge cooled in liquid nitrogen or propane, cooling rates are usually limited not by the liquid but by the cold gas layer that forms above it. By removing this cold gas layer, cooling rates can be increased by a factor of 10 or more, and glycerol concentrations required to eliminate crystallization in protein-free mixtures can be reduced by a factor of four or more. For many proteins, faster cooling may allow penetrating cryoprotectants to be eliminated from cryopreservation protocols.

M. Warkentin, V. Berejnov, N. S. Hussein and R.E. Thorne

X-ray intensity fluctuation spectroscopy by heterodyne detection

J. Synchrotron Rad. (2006). **13**, 453–458 [doi:10.1107/S0909049506030044]



Oscillatory behavior of the speckle correlation function for various angles between the diffraction vector and the drift direction (velocity: 1.5 nm/s) of the relaxing rubber. The frequency of this oscillation is the Doppler shift of the X-rays scattered from the rubber

Heterodyne measurements coherently mix a reference signal with the signal from a sample, giving access to relative phase. A demonstration experiment shows how the local microscopic velocity in a rubber relaxes after stretching. Heterodyning gives an oscillatory intensity leading to a map, in reciprocal space, of how the velocities of the filler particles in the rubber evolve. The method distinguishes between mechanical relaxation and the local motion of the aggregates. The resulting dynamics appear to be related to a recently recognized characteristic of crowded systems, jamming.

F. Livet, F. Bley, F. Ehrburger-Dolle, I. Morfin, E. Geissler and M. Sutton

MEETING REPORT

SESAME a bright light of hope to the Middle East



The 5th SESAME Users' meeting was held in Alexandria, Egypt November 29 - December 2, 2006.

Alexandria, overlooking the Mediterranean Sea, has been, and continues to be, one of the world's most significant melting pots for different cultures, religions and races.



SESAME building, Jordan. Photos courtesy of R. Sarraf, Al-Balqa-Applied U.



SESAME stands for **S**ynchrotron light for **E**xperimental **S**cience and its **A**pplications in the **M**iddle **E**ast. It is a synchrotron facility which is being built in Jordan under the auspices of UNESCO. Currently, the full members of the project are Bahrain, Cyprus, Egypt, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey. Moreover, France, Germany, Greece, Iran, Italy, Kuwait, the Russian Federation, Sweden, the United Arab Emirates, UK and US will act as observers.

Starting in the year 2000, scientists from the region began meeting in a series of scientific workshops (see reports at www.sesame.org.jo). Annual SESAME Users' meetings began in Jordan in 2002 followed by Iran in 2003, Turkey in 2004, and back to Jordan in 2005.

The success of the four previous Users' meetings was clearly reflected in the number of applications for the 5th user meeting in Egypt. More than 200 applications were received from 18 countries. In attendance at the meeting, were about 55 local participants from different universities and research organizations in Egypt as well as scientists from Algeria (4), Jordan (15), Israel (3), Pakistan (7), Turkey (8), Palestine (3), Italy (3), Canada (1), the UK (3), the UAE (2), Bahrain (2), the USA (5), Yemen (2), Syria (2), France (5) and Germany (4). Official invitations were also sent to several scientists from Iran. Unfortunately, due to longer than expected procedures, they could not get their visas on time.

Representatives from the International Atomic Energy Agency (IAEA) and the Canon Foundation were present. The participation of William Duax, the immediate past president of IUCr was also notable and highlights the attention that the SESAME project has been receiving.



Bibliotheca Alexandria, site of the 5th SESAME Users Meeting. Photos courtesy of Dale Tronrud



The meeting was sponsored and supported by UNESCO, the Academy of Scientific Research and Technology of Egypt, the Faculty of Science of Cairo University, Bibliotheca Alexandria, the US Department of Energy (DOE), the Office of External Activity (ICTP, Trieste, Italy), the Canon Foundation (London, UK) and the IUCr.

The meeting was preceded by a joint session of the SESAME Beam Lines and Scientific Advisory Committees and followed by a workshop on Synchrotron Applications in Macromolecular Crystallography.



Minster Hany Helal (middle) is greeting Herwig Schopper (left) and Tarek Hussein (right).

The opening session on November 29 was chaired by Schopper, President of the SESAME council. Tarek Hussein, President of the Egyptian SESAME Committee gave a welcoming note followed by Herwig Schopper who spoke about the status and future prospects for SESAME and finally Hany Helal, Minister of Higher Education and Scientific Research (Egypt) concluded with a promise of Egypt's continuing commitment to the success of SESAME. This session was followed by presentations by Aslam Baig (Scientific director of SESAME) who spoke about the scientific directions of SESAME, Maged Al-Sherbiny (Cairo University and a member of the SESAME Scientific Committee) who outlined Egypt's vision for SESAME, Zehra Sayers (Chairman of the SESAME Scientific Committee) who discussed the role of SESAME members in the construction of Phase I beam lines and Herman Winick (Stanford Synchrotron Radiation Lab (SSRL), one of the founders of SESAME) who talked about the impact of synchrotron related research on developing countries.



Minster Helal talking to Samar Hasanain during the coffee break

The users meeting lasted for three days and covered many different scientific disciplines. The scientific themes for the first day were material science, nanotechnology, structural biology and drug design.

Zahid Hussain (Pakistan/USA), Giuseppe Dalba (Italy), Awni Hallak (Jordan), Samar Hasanain (England), Irit Sagi (Israel), Paul Tucker (Germany) and Dan Tawfik (Israel) were the main speakers.



Maged Al-Sherbiny



Zehra Sayres

In the morning of the second day, all participants were invited to the Antique and Manuscript museum at Biblotica Alexandria. In the afternoon, the scientific program continued with talks on the environment and archeology. Faridah Jalilehvahd (Canada), Paul Dumas (France) and Phillip Walter (France) were the major speakers.

The scientific themes for the third day were physics and engineering, medical and biological sciences. Martjin Fransen (Netherland), JP Connerade (France/UK), Amina Taleb-Ibrahim (France), Maged Al-Sherbiny (Egypt), Ahmed Elbedawi (Egypt), Mohammad Yousef (Egypt/Japan) and Abdel Maged Mamoon (Egypt) were the main speakers. Every session in the meeting was followed by short presentations on proposed projects.

In the concluding session, Zehra Sayers announced that positions are available for two beam line scientists and Francoise Muelhauser (IEAE) described a training program funded by IEAE for beam line scientists. Many points were discussed and recommended, most importantly, the formation of collaborative groups among SESAME members in different disciplines and also consortia of countries to build the Phase I beam lines.

Tarek Hussein said that Egypt will establish a central SESAME lab for sample handling and computational analysis. The center is expected to be a state-of-the-art facility linked to the SESAME project to serve and train scientists from the entire region.

The next SESAME Users' meeting is planned to be held in the new SESAME member country of Cyprus in September 2007.



Zahid Hussain (left) with Mohammad Yousef.

Against all odds, and due to the sincerity, dedication and persistence of a devoted team, SESAME is now a living reality. It stands as an outstanding opportunity to promote science and technology in the Middle East as well as to promote mutual understanding and cooperation. The beamlines will be a bright light of hope for many young scientists in the region. However, as the project moves from being wishful thinking to the actual beginning of phase I design and construction, important questions remain. How big is the “ready to go” user community? What are their needs? What are the factors that will help them work together? What is the availability of qualified staff, budget and commitments? These issues might be the themes of the next user meetings.

For more information about SESAME, visit www.sesame.org.jo.

Mohammad Yousef, Maged Al- sherbiny and Tarek Hussein, Cairo U., Egypt

MEETING REPORT

Workshop on the application of synchrotron radiation in macromolecular crystallography

Cairo, Egypt, November 29 - December 2, 2006



Herman Winick (An early proponent of SESAME)

The objectives of this workshop were to:

- Expose the scientific community (especially students) in Egypt and SESAME member countries to the practical aspects of macromolecular crystallography. The hope was that through such exposure, the value of the technique will be appreciated and an interest in the field will be developed and propagated.
- Show that developing SESAME labs in each member state is feasible especially for crystallization, data processing and analysis.
- Start a nucleus for a SESAME lab in Egypt for sample preparations and computational analysis.



Dale Tronrud (trying to run CCP4 on an unfamiliar Linux)

Mohammad Yousef coordinated the workshop. With the help of the scientific committee, he put together a program of lectures and practical sessions, chose the speakers and arranged for needed materials and software. The program consisted of three days of lectures (morning) and practical sessions (afternoon). The first day focused on sample preparation and crystallization, the second day covered data processing and analysis, and the third day was spent on refinement, model building and bioinformatics. The faculty of Science, Cairo University provided a modern wet lab and a well equipped computational facility for the workshop. Dale Tronrud (USA), Paul Tucker (Germany), Bill Duax (USA), Robert Heuther (USA), Zain Heba (Egypt), Said Abdelfattah (Egypt), Mohammad Yousef (Egypt/Japan), and Herman Winick (USA) were the main speakers.



Hands-on experiment, sample handling and protein crystallization

The practical sessions were very successful. The students, for the first time in Egypt and the Arab world, were able to experience the different steps of a protein crystallography experiment. They started with

the crystallization of hen egg white lysozyme and proceeded to data analysis and model building. The students worked in groups of 2-3 persons to allow them sufficient “hands-on” experience. Bill Duax and Robert Heuther gave lectures and practical sessions on Bioinformatics that attracted a lot of attention. Many thanks are due to Dale Tronrud who was critical to the success of the workshop. He was instrumental in setting up the hardware and installed, tested and ran the software. He also gave two insightful lectures.



The bio-computational lab in the Faculty of Science, Cairo University. Dale Tronrud is in the far front. Follow up and future plans: The computational and wet labs used for the workshop are the first step in the establishment of a SESAME center of excellence in Egypt. More than a dozen highly qualified students showed interest in continuing their graduate career in the field of synchrotron science. Arrangements will be made to start them on masters or Ph.D programs with the available resources.



Mohammad Yousef helping students process X-ray diffraction images.

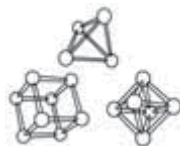
In the workshop, students learned how to use the programs needed to process synchrotron data on protein structures and attempt structure determination. Any crystallographer in the world who would like to support the SESAME project and is willing to provide unprocessed synchrotron data on a protein to beginning crystallography students in Egypt or other SESAME member countries should contact M. Yousef (yousef@post.kek.jp). Data on solved, published structures would be useful as exercises, but data on unsolved structures could be the basis for international collaboration and a richer, more rewarding, exercise.

Mohammad Yousef and Tarek Hussein

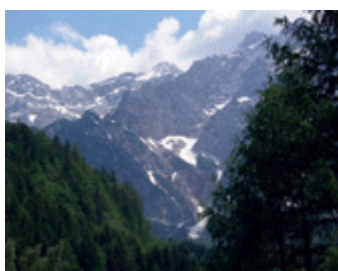
MEETING REPORT

15th Slovenian-Croatian crystallographic meeting

Slovenia, June 2006



The Meeting was held in Jezersko, a small village thought to be the most beautiful place between two mountain ranges, Karavanke and Kamnik-Savinja Alps. It lies some 900 meters above sea level in a peaceful area surrounded by Alpine peaks high enough to still be covered with snow during the Meeting.



There were 68 active participants and 15 accompanying persons from eight countries. His Excellency, The Ambassador of Croatia to Slovenia, Mario Nobilo, took part in the opening ceremonies. Forty four short oral contributions were presented on contemporary topics in crystallography.

L. Golic (Ljubljana) and B. Kamenar (Zagreb) were the honorary chairs of the Meeting. I. Leban (Ljubljana) and S. Popovic (Zagreb), the programme co-chairs, have been working on these meetings since the first one 15 years ago. Special thanks are also due to the members of the Organizing Committee: N. Lah, V. Kaucic, A. Prodan and A. Meden.



The Slovenian Crystallographic Society and the Croatian Crystallographic Association are determined that future meetings will be held with the same concept of no registration fees and primarily oral presentations. The book of abstracts for this meeting contains a list of plenary lectures presented at all 15 meetings.

We would like to express our gratitude to our sponsors and donors: the Ministry of Higher Education, Science and Technology of Republic of Slovenia; the Slovenian Research Agency; the faculty of Chemistry and Chemical Technology, University of Ljubljana; Micro-Polo d.o.o., Maribor, Slovenia (distributor for Bruker AXS GmbH); RENACON d.d., Zagreb (distributor for PANalytical); SCAN d.o.o., Preddvor, Slovenia (distributor for JEOL), the Cambridge Crystallographic Data Centre; Rigaku, Europe; Oxford Diffraction Ltd; Marresearch GmbH; Oxford Cryosystems Ltd; and Medis d.o.o., Ljubljana.

The next meeting will be held in Croatia in June 2007, in a resort on the Adriatic Coast. For more

information or to be put on the mailing list, contact S. Popovic, spopovic@phy.hr, or I. Leban, ivan.leban@fkkt.uni-lj.si.

Ivan Leban, Slovenian Crystallographic Society



From left: Anton Tonejc, Davo Karnicar and Ivan Leban.

It is encouraging that in a world increasingly fragmented by artificial national, ethnic, religious and language barriers crystallographers from several countries can come together to discuss crystallography and enjoy each other's company in an atmosphere of scenic beauty. There were four plenary lecturers, one each from crystallographers in Slovenia and Croatia and two from abroad. Robert Dinneber (Germany) reviewed recent advances in powder diffraction and illustrated how one can determine the structure of numerous temperature dependant phases of a compound in a single experiment with synchrotron radiation. Marija Kosec (Ljubljana) presented a comprehensive review of her powder diffraction and XAFs studies of the dielectric, pyroelectric, and piezoelectric properties of ferroelectric ceramics and their use in industrial applications for process control, environmental monitoring, information systems, and medical instrumentation. G. Stefanic (Zagreb) described the formation of high temperature ZrO_2 polymorphs at room temperature and the importance of these strong, chemically resistant materials for use in cutting tools, automotive engine parts and valve seals. William Duax (USA) spoke on "The genes, amino acid sequences and crystal structures of short chain oxidoreductase enzymes". Dozens of ten-minute presentations covering the gamut of crystallographic application from minerals to macromolecules using powder, single crystal and small angle scattering techniques. Each of the speakers managed to illustrate interesting new chemical, physical and biological information derived from their crystallographic structures. Andreja Zaga (The Netherlands) described the first crystal structure of a glucansucrase of particular interest for its agricultural importance. Dalibor Milic, (Zagreb) is pursuing the determination of the human serum apotransferin (apt). The structures of hen, rabbit and pig apt have been reported but it has proven difficult to crystallize the human form. The 40% sequence identity and structural similarity of the N and C terminal halves of apt reflected in the three dimensional structures suggests that they are the product of gene duplication.

Several talks focused on using powder diffraction to study antiquities including bronze statues in the Adriatic Sea (Stanko Popovic, Zagreb) the materials used to coat the external walls of the manor house Novo Celje (Mit Dobnikar, Ljubljana), and fragments of Pottery found near Belgrade (Darko Tibljars, Zagreb). New techniques for crystallization of zeolites from gels and their analysis by high resolute transmission electronic microscopy and as well as Xray diffraction were well described and beautifully illustrated (C. Kasonovic, Ljubljana). The chemistry involved in the inclusion of ion in the zeolites was also discussed (S. Bosnar, Zagreb). Anton Meden (Ljubljana) gave a fine example of determining the structure of a Mo-S-I nanowires that provided only two-dimensional data from which he teased a convincing three-dimensional structure. He used a handful of hexagonally shaped pencils to illustrate the model to good effect.

M. Fleck (Austria) has begun a thorough examination of the most essential biological molecule Glycine. He is studying of series of crystal structures in which Gly is present as a monodentate, bidentate, tridentate or bridging ligand. Of particular interest are chiral crystals in which the glycine molecule is either pro R or Pro S. His studies indicate that in all chiral crystal forms, complexation has led to a chiral selection. All crystals from a given sample have the same chiral form (all Pro R or all Pro S). This study may contribute to a new explanation of why we live in a world of proteins with L-chirality.

Kresimir Molcanov (Zagreb) who seems to do his best work around Valentine's Day described assemblies of macrocyclic thialactones included a compound that takes up the shape of a heart when crystallized around February 14, but has alternate forms for other seasons. The heart shaped molecules are linked by C-H...O hydrogen bonds.

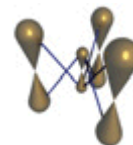
In a new study of cholic acid host/guest complexes Goron Stefanic (Zagreb) drew attention to a consistent pattern of P , crystallization in the space group $P2_1$ with an $8.01 \pm 0.2 \text{ \AA}$ b cell dimension in a series of complexes of extremely variable size and composition. He did not offer an explanation but hopes to have one by next year's meeting in Croatia.

A field trip to Brdo, a baroque castle provided a pleasant afternoon of strolling in wonderful wooded grounds. Enthusiasm for the castle was tempered by the fact that it had been a private residence of Tito, that the German force had occupied it during the war, that Prince Andrew of Monaco had dined there. We were told that the Slovenian crystal in the castle was so wonderful that it needed to be protected from large groups such as ours. Perhaps most disconcerting was the fact that George Bush and Vladimir Putin had met there 5 years to the day before our visit.

William L. Duax

MEETING REPORT

Indaba 5

Berg-en-Dal, Kruger National Park, South Africa, August 21-25, 2006

Over 70 delegates from all corners of the globe converged on the Berg-en-Dal rest camp in the Kruger National Park to attend the fifth Indaba of the South African Crystallographic Society, a meeting that is sponsored by the IUCr Commission on Structural Chemistry. The theme of the workshop, “Models, Mysteries and Magic of Molecules”, provided opportunities for a rich diversity of topics to be discussed, from the fundamental nature of a molecule to the engineering and properties of molecular crystals and proteins. This was in keeping with the “Indaba “ spirit, i.e. to study a subject in depth from a number of different angles. The scientific program consisted of 42 lectures and 26 posters. Upon arrival delegates were delighted to find a complimentary copy of the book, “New Theories for Chemistry” by Jan Boeyens, (sponsored by Bruker SA and Elsevier) included in their conference pack. Few realized that they were expected to read it before the first talk on Monday morning.



Jan Boeyens and Yuji Ohashi at Indaba5

After starting the conference with an early morning game drive, Dave Billing, President of the South African Crystallographic Society, welcomed the delegates to the unique bushveld venue. Yuji Ohashi (Hyogo), President of the IUCr then opened the proceedings with a short review of the structure and activities of the Union, after which Jan Boeyens (Pretoria) gave an overview of the theories underpinning our understanding and misconceptions of atoms and molecules. This ranged from a description of the Bohr atom and the myth of hybrid orbitals to the holistic nature of the molecule, setting a new direction for theoretical chemistry.



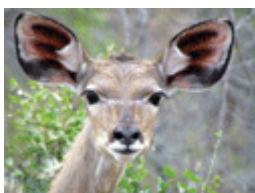
Participants at Indaba 5

Highlights from the four full days of lectures included: Hans-Beat Bürgi (Bern) who gave a superb account of the information lost in some structures when considering only the Bragg positions in a talk

entitled “Loss of translation - Lost in translation”. Later, Jan Dillen (Stellenbosch), expounded the features of donor-acceptor complexes in a talk “Mock or Marvel? The Metamorphosis of the Dative Bond.”.



Jumping to a different viewpoint John Helliwell (Manchester) addressed a puzzling question: “Why do lobsters change from blue/black to red on cooking?” The answer to this is far from trivial, as he explained in his talk “Unravelling the mechanism of the bathochromic shift in the lobster carapace; the protein crystal structures of Crustacyanin in its Carotenoid bound and unbound forms.” In another protein structure related project, Martin Egli (Nashville) provided new insight into the clocks that drive our natural biorythms in his contribution, “Protein-Protein Interactions in the Cyanobacterial KaiABC Circadian Clock.”



Leaping onto other planets, have you wondered if there is life on Mars? Howell Edwards (Bradford) explained what strategies and techniques we could use to probe such extreme environments in a fascinating talk on “Raman Spectroscopy: The biomolecular detection of life in extreme environments.”



Zorka Papadopolos (Tübingen) reminded us of our limitations in working in only three dimensions when describing quasicrystals, “Clusters in icosahedral quasicrystals.” and Peter Comba (Heidelberg) explained how one gets different answers to questions relating to accurate structure prediction versus techniques to understand properties of Jan-Teller isomers of bispidine complexes. “Models for isomeric bispidine complexes and their properties. Accurate prediction vs. thorough understanding.”

John Ogilvie (San Jose) surprised some delegates when he stated that a molecule in a quantum state has no size, no shape, and no extension in space or time: The structure of a molecule is the result of the environment. “Unravelling the mysteries behind theoretical and experimental models of molecules.”

Mihail Atanasov (Sofia) continued the theoretical perspective of the conference by questioning the ligand field paradigm with his talk: “The ligand field paradigm and new insight into the electronic properties of transition metal complexes based on modern electronic structure calculations.”

The proceedings then swung toward scientists addressing polymorphism and co-crystallization. Joel Bernstein (Beer Sheva) gave an elegant account of attempts to generate co-crystals containing the R₄,2(8) hydrogen bonding motif that yielded instead unpredictable polymorphs in his talk simply entitled “Co-crystals and Serendipity” .

Elena Boldyreva (Novosibirsk) explored the magic of amino acids in a fascinating talk on “Polymorphism of crystalline amino acids - a link between chemistry, materials science and biology.” During her talk she

also reminded delegates that “Indaba is the only meeting where dreaming is allowed and even encouraged”.

The final talk was given by Gautam Desiraju (Hyderabad) who philosophised on the parallel between the mysteries of nature and the mysteries of molecules and crystals, while listing his view of five major future challenges in crystal engineering.

The poster session on the Tuesday evening was well attended, with lively discussion facilitated by the free South African wines. Two poster prizes were awarded during the closing ceremony. One, sponsored by the RSC was awarded to Simon Iremonger (Sydney) for his poster “Porous Homochiral Metal-Organic Frameworks” and the second, sponsored by CrystEngComm was awarded to Melanie Rademeyer (Pietermaritzburg) for a poster “Non-covalent interactions in 2-phenylethylammonium perhalometallates”.

At the closing ceremony Alessia Bacchi (Parma) chair of the Commission on Structural Chemistry, thanked the organizing committee. Jan Boeyens, founder of the Indaba conferences, made some comments and put the Indaba series into historical perspective, pointing out that the five Indabas to date have had a strong support from the IUCr: four IUCr presidents have attended (Philip Coppens, Henk Schenk, Bill Duax, and Yuji Ohashi) and three chairs of the CSC (Lee Brammer, Judy Flippen-Anderson; Alessia Bacchi). Jan also acknowledged the contributions of two other founding members who could not be present, Ivan Bernal and Anton Amann.

Peter Comba gave an amusing and insightful view of the proceedings in his closing talk, with a quip on the biological rhythms cited by Martin Egli, stating that “Your answer to the question whether all biological clocks have a 24 hour cycle was wrong. My clock is different, it has a 3 year cycle: Now is INDABA time, from tomorrow onwards it is either after or before the next INDABA time. (the Indaba is held every three years).

Finally Dave Billing introduced the new “Big Five Awards” for attendance of the Indabas, and presented gifts to Jan Boeyens, Peter Comba and Demi Levendis who have attended all five Indabas; Gert Kruger, John Ogilvie and Manuel Fernandes who have attended four of the Indabas.

The organizers would like to thank the sponsors: IUCr, Bruker, South African National Research Foundation, RSC, CrystEngComm, CCDC, Elsevier, Microsep, Universities of Pretoria, and the University of Witwaterstrand.

In retrospect, Indaba V managed to fulfill its goal of being a highly stimulating and successful “meeting of minds”, and judging by the selection of pictures posted on the website (mating lions: www.sacrs.org.za/indaba5/) the game viewing was as satisfying as the meeting.

Demi Levendis

OBITUARY

Desmond Cunningham (1942-2006)



Des Cunningham, who died on September 18, 2006, was a Chemistry Professor at the National University of Ireland, Galway. His passing represents a loss for the chemistry and crystallographic community in Ireland. His research, (with more than 175 papers), focused principally on the synthesis and characterisation of Group 14 derivatives using Mössbauer spectroscopy and X-ray diffraction techniques, made him a key figure in the development of Inorganic chemistry in Ireland since the 1970s.

He was born on March 6, 1942 and grew up in Mountcharles in County Donegal. In his early years both music and painting competed with his interest in science. He was educated at University College Dublin where he studied synthetic inorganic chemistry (1965-1968). He did his PhD work on 'Studies of Chromium(III) Alkoxides' at the National University of Ireland under the supervision of W. K. Glass.

Post-doctoral research in London, in the then Northern Polytechnic, introduced Des to the chemistry of tin which became a life long interest in conjunction with Mössbauer spectroscopy. In 1971 he moved to University College Galway and established a thriving research group engaged in the study of Group 14 and transition metal complexes.

Des had a strong interest in solid state chemistry and had often dreamed of establishing a crystallography group in Ireland. In the late 1970s he spent a sabbatical year in Oklahoma, USA where he gained considerable expertise in using diffraction equipment and running a crystallography laboratory. From this experience the Crystallography Centre in Galway was established with collaboration from Patrick McArdle and Tim Higgins. Initially a Hilger & Watts Y290 4-circle diffractometer was used for data collection (from George Ferguson, University of Guelph, Canada). The positive impact of this diffractometer was immediate, driving research in new directions in synthetic and structural chemistry both in Galway and in collaboration with other Irish research institutions. Two successive HEA large equipment grants provided further funding for more modern equipment to expand research in chemical crystallography, powder diffraction and biological crystallography.

A pharmaceutical company in Ireland had a problem with a tin catalysed reaction using a process that produced the desired drug in one hour but left a tin oxide 'mess' that took many hours to clean up. Des and co-workers overcame the problem using inexpensive chemicals by turning the 'mess' into a white powder that was easier to handle. Production was tripled in all plants in which the drug was produced (which represented >20% of the companies worldwide profits). Together with coworkers he patented a superior process for coating glass with tin and other metal oxides. These very thin oxide coatings make plate glass windows and glass bottles much stronger than uncoated glass.

During his recent illness he was always optimistic and continued to involve himself in correcting theses and suggesting reactions from his hospital bed. Several fascinating compounds were synthesised by his research students and their crystal structures solved and examined by him in the days before his death.

Des thought well of everyone and he had more friends than most. The wonderful atmosphere he created with his personality, his music and his love of painting will long be remembered. He appreciated a well poured pint of stout amongst friends - a life long interest which hadn't diminished with age. He was an

excellent teacher, mentor and friend to the many students he taught as undergraduates or supervised as postgraduates as well as his colleagues and friends.

Des, a dedicated family man is survived by his wife Patsy, his daughter Aileen, his brother Conal and his sisters Shelia and Catherine.

Patrick McArdle, John Gallagher, and John McGinley

OBITUARY

Yoichi Iitaka (1927-2006)

Yoichi Iitaka, Emeritus Professor of the University of Tokyo, died on April 1, 2006 after struggling against cerebral hemorrhage for several years. He was born in 1927 in Yamanashi Prefecture in central Japan. He was educated and worked at the University of Tokyo. After receiving his Ph. D. degree in 1959, he studied the structures of inorganic and mineral crystals in Britain and Switzerland before becoming an Associate Professor in the Faculty of Pharmaceutical Sciences of the University in 1961. During this period he discovered and determined two new crystal forms of glycine. From 1967 to 1988, he taught students structural and analytical sciences, and carried out X-ray crystallography research. He also held a professorship at the Teikyo University of Science and Technology until his retirement in 1997.

He was quiet but full of deep and ardent insight into the structural sciences. He started with mineralogy, and went on to determine the structures of many important biological molecules, including peptides, nucleic acids, antibiotics, natural products, organic and medicinal compounds, and mutagenic substances. He extended his research to include biological macromolecules, determining the structures of such proteins as microbial ribonucleases, and the proteinase inhibitor SSI as well as its complex with subtilisin BPN'.

He was active within the crystallographic community in Japan successively serving as a member of the Japanese Crystallographic Society Council and the Japanese National Committee for Crystallography over a period of 25 years. He contributed to the success of IUCr Kyoto Conference in 1972, and served as Society President in 1985. He was very good at crystallographic instrumentation, building detectors and diffractometers. From the early days of crystallographic computing, he directed his efforts toward the development of computer software, hardware, and databases. He contributed to the establishment and organization of large-scale computing facilities for Japanese universities and the synchrotron radiation facilities of the Photon Factory of KEK.

Yoshinori Satow, satowy@mol.f.u-tokyo.ac.jp

OBITUARY

Elizabeth Armstrong Wood (1912-2006)

Following a very active life filled with many interests, Elizabeth A. Wood died March 23, 2006 of a stroke about a month after a pacemaker was installed. Born October 19, 1912 in New York City, she earned her BA at Barnard College and her MA and PhD in geology at Bryn Mawr College. Her growing enthusiasm for crystallography was encouraged by A. Lindo Patterson who was then in the Bryn Mawr Physics Dept. Betty became an instructor in geology at Bryn Mawr from 1934 to 1935 and again from 1937 to 1938. She was also an instructor in geology and mineralogy at Barnard from 1935 to 1937 and from 1938 to 1941, becoming a research assistant at Columbia U. before joining the Physical Research Dept. at Bell Telephone Laboratories (BTL) in 1942 where she was the first woman scientist. She maintained an active crystallographic research program for the next 24 years at BTL.

Her interests ranged from the growth of single crystals with useful semiconducting, lasing, magnetic or superconducting properties to the crystallographic investigation of new materials with unusual properties such as the exhibition of both ferromagnetism and piezoelectricity. She also worked on material phases that could be changed by the application of appropriately oriented electric fields and on the formation of new superconductors. The ability to walk down the corridor and consult with a world authority on almost any aspect of physics was a BTL hallmark; Betty was one whose advice was regularly sought by many of the most inventive minds at BTL including B.T. Matthias, W.L. Bond, R.M. Bozorth and L.H. Germer among others who are less well known to crystallographers.

As secretary of the American Society for X-Ray and Electron Diffraction (ASXRED) in 1947 Betty, together with William Parrish who was secretary of the Crystallographic Society of America (CSA), issued an invitation to the newly formed IUCr to hold their first Congress and General Assembly in the US at Harvard. She met with other officers of ASXRED and CSA during the Congress to explore the possibilities of a merged society. Their resulting proposals were accepted by both societies, but not without vigorous discussion as feelings on the plan ran surprisingly high. The following year she, Isadore Fankuchen, Bill Parrish and Lindo Patterson drafted a Constitution for the proposed American Crystallographic Association. In 1957, she became the first woman president of the ACA; the second, Isabella Karle, was not elected until 1976.

She chaired the US delegation to the second IUCr General Assembly in 1957 and was a delegate to the tenth. She served on the Governing Board of AIP from 1963 to 1969, was on AIP's Visiting Scientist in Physics program 1961-1972 and the Commission on College Physics 1967-1971, and was Associate Director of the NSF project Physical Science for Nonscience Students 1965-1971. She was also an Advisory Board member of the School of Mathematics Study Group 1966-1969 and a member of the IUCr Commission on Crystallographic Teaching 1969-1972. A Fellow of the American Physical Society, she was also a member of AAPT, AAAS, Sigma Xi and the NJ Science Teachers Association. She was awarded a D.Sc. (*honoris causa*) by Wheaton College in 1963, Western College, Ohio in 1965 and Worcester Polytechnic in 1970.

Her reputation for clearly written texts spread as a result of her *Rewarding Careers for Women in Physics* (1962) and *Pressing Needs in School Sciences* (1969) published by the American Institute of Physics (AIP) in 1962. It became wider still with the publication of her *Crystal Orientation Manual* in 1963, which

expounded the art and science of preparing shaped pieces of large accurately oriented single crystals for technicians and her 1964 *Crystals and Light: An Introduction to Optical Crystallography* under the auspices of the Commission on College Physics, written for students with no previous knowledge of crystals or light. That same year, *Experiments with Crystals and Light* came out in the Bell System High School Series as both a booklet and a kit. Five years later, her *Science for the Airplane Passenger* was published and proved very successful, appearing for many years in airport bookstores throughout the US and other countries. Her deep interest in improving the scientific understanding of the general public was recognized by the ACA's establishment of an Elizabeth A. Wood Science Writing Award. Its purpose is to honor the authors of outstanding publications that bring science to the attention of the general public. The first award was presented in 1997 to Nobel laureate Roald Hoffmann.

Betty's interests were not confined to science. For many years, she and her husband Sandy hybridized and raised the most beautiful irises in their large Murray Hill garden. She was elected president of the Garden State Iris Society and the Median Iris Society. She loved ocean sailing, putting her sailboat to regular use until a year or so ago. She was also a skilful thespian both as actor and playwright. Her other interests included recording numerous textbooks for the blind over many decades. Her warmth and outstanding presence will be sorely missed by her many friends.

Sidney Abrahams, ACA RefleXions, Number 2, Summer 2006