

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



In 1948, the IUCr held its first General Assembly and Congress at Harvard University, Cambridge, Massachusetts, USA. Only 310 crystallographers attended and 83 papers were presented. There were only four Adhering Bodies: Canada, Norway, UK and USA. The history of the IUCr is clearly described by D.W.J. Cruickshank in an article that forms the first chapter of *Crystallography Across the Sciences*, a Special Issue of *Acta Crystallographica* Section A [*Acta Cryst.* (1998), **A54**, 687-696] edited by H. Schenk and published in celebration of the 50th anniversary of the IUCr in 1998. This article is also available from the IUCr web pages (www.iucr.org/iucr-top/iucr/dw/sc0025.html).

Since then, 60 years will have passed by the time of the next IUCr Congress to be held at Osaka, Japan, in 2008. The number of the participants is expected to be 3,000 and the number of Adhering Bodies is now 40. Both numbers are ten times larger than those at the time of the Harvard Congress. Moreover, the IUCr now publishes eight scientific journals; of these, *Acta Crystallographica* Sections A and B and the *Journal of Applied Crystallography* will have been published for 40 years in 2008. At its meeting in Leuven this summer the Executive Committee decided to hold some commemorative events celebrating both the 60th anniversary of the IUCr and the 40th anniversaries of *Acta A*, *Acta B* and *JAC*.

The first will be the publication of a Special Issue of *Acta A* as the first issue of 2008. The papers will be reviews with a personal touch and emphasize the influence of crystallography in different fields of research. The entire issue will be open access making it freely available on the web. Henk Schenk has agreed to edit this Special Issue in collaboration with the Editor of *Acta A* (Dieter Schwarzenbach) and the Editor-in-Chief (Gernot Kostorz). 30 potential authors have already been contacted. The second celebration will be a 60th Anniversary Ceremony, Crystallography in Life, to be held in Osaka just before the Opening Ceremony of the 21st General Assembly and Congress in 2008 to highlight how much crystallography has contributed to human development. Several crystallographers, including Nobel Prize laureates, will be invited to make presentations at the ceremony. The President and the Executive Committee are making the plans.

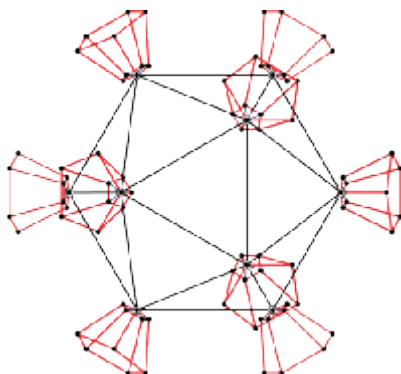
The third is a photographic exhibition. Over the years Bill Duax has taken many photographs, not only at IUCr Congresses but also at many local or special crystallographic meetings. Chris Gilmore, Gernot Heger and Syd Hall also have many photographs involving the Regional Associates and other specialized meetings and the Chester office has photographs from the early days of IUCr. Selected photographs will be exhibited in a special room at the Osaka Congress.

None of these events will be successful without useful suggestions from crystallographers all over the world. The Executive Committee heartily welcomes constructive suggestions for the celebratory events mentioned above.

Yuji Ohashi, yohashi@spring8.or.jp

Towards a classification of icosahedral viruses in terms of indexed polyhedra

***Acta Cryst.* (2006). A62, 319-330 [doi.org/10.1107/S0108767306022227]**



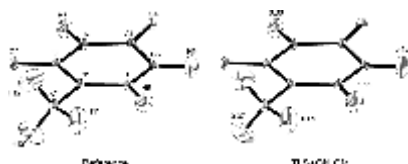
Icosahedron with vertices decorated by truncated pentagonal pyramids. The generating points are at $[600000]$, $[711111]$ and $[111333]$. This decoration could be a model for viruses with protruding proteins like the spiroplasma virus.

The standard Caspar-Klug classification of icosahedral viruses and Twarock's Penrose-like characterization of strains not obeying the Caspar-Klug rules are special cases of an approach based on polyhedra having vertices indexed by icosahedral lattice points. Icosahedral rotations combined with scalings leaving the icosahedral lattice invariant (linear, planar, and 3-dimensional) permit edge, face and vertex decoration. In the last case satellite polyhedra are attached to the vertices of a central polyhedron. In all cases the whole is generated from a set of points with rational indices.

A. Janner

Anisotropic displacement parameters for H atoms using an ONIOM approach

***Acta Cryst.* (2006). B62, 875–888 [doi.org/10.1107/S0108768106020787]**



ORTEP comparison between TLS+ONIOM and neutron ADPs for 1-methyluracil at 21 K (99% surfaces). Numbers are values of a similarity index that measures overlap between reference and model probability density functions.

Charge-density analyses of molecular crystals require an accurate description of the motion of all nuclei, including hydrogens, yet nearly 80% of recent studies treat motion of hydrogen atoms isotropically. Using widely available software we combine *ab initio*/molecular mechanics ONIOM cluster calculations with rigid body fits to X-ray ADPs for heavy atoms, to derive ADPs for hydrogens for a variety of molecular crystals. The agreement with neutron diffraction results is impressive, and the method offers considerable promise in future charge-density studies of molecular crystals.

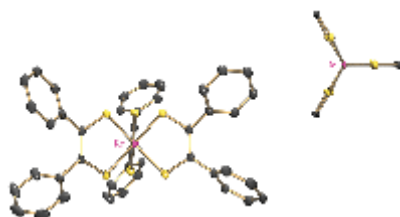
A.E. Whitten and M.A. Spackman

IUCR JOURNALS NEWS

Redetermination of the trigonal prismatic complex tris(*cis*-1,2-diphenylethylene-1,2-dithiolato)rhenium

Redetermination of the trigonal prismatic complex tris(*cis*-1,2-diphenylethylene-1,2-dithiolato)rhenium

***Acta Cryst.* (2006). C62, m464-m466 [doi.org/10.1107/S0108270106033336]**



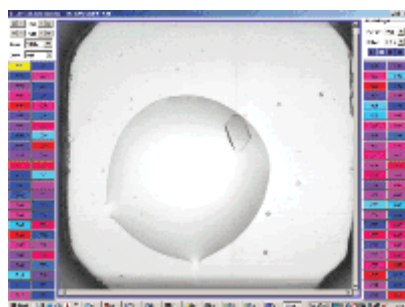
The first structurally characterized example of trigonal prismatic coordination reported forty years ago, $\text{Re}(\text{S}_2\text{C}_2\text{Ph}_2)_3$, was redetermined from the same sample using modern CCD instrumentation. The results confirm the original determination, albeit with better agreements among bond distances and angles and without using a group refinement for the phenyl rings. A survey of related MS_6 molecules reported over the years is included that assesses the degree of trigonal prismatic coordination using a designated dihedral angle for comparison.

R. Eisenberg and W.W. Brennessel

IUCR JOURNALS NEWS

SPINE high-throughput crystallization, crystal imaging and recognition techniques: current state, performance analysis, new technologies and future aspects

***Acta Cryst.* (2006). D62, 1137-1149 [doi.org/10.1107/S090744490602943X]**



An image of a crystal from a nanoliter crystallization trial in a development version of the PIMS crystallization management system. Figure courtesy of Dr. J.M. Diprose (unpublished work).

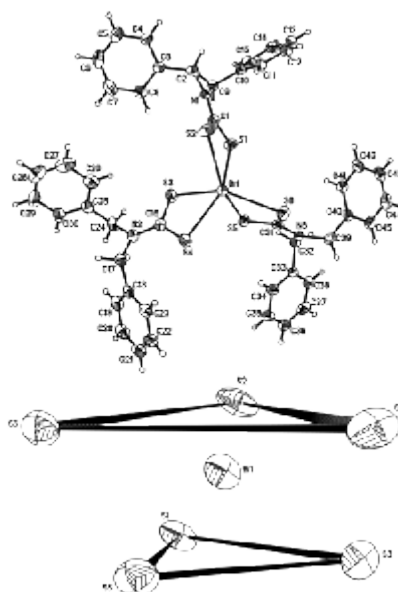
An outstanding outcome of the EU funded project SPINE (Structural Proteomics In Europe) is the establishment and advancement of high-throughput nanoliter crystallization, crystal imaging and recognition techniques in the partner laboratories of the consortium. The uptake, use and experience of the new technologies by SPINE partners across Europe have been surveyed and a picture emerges of highly successful adoption of novel working methods revolutionizing this area of structural biology. In general, the introduction of automation and miniaturization into crystallization workflows has resulted in the growth of a greater number of high-quality crystals for a wider variety of proteins.

I. M. Berry, O. Dym, R. M. Esnouf, K. Harlos, R. Meged, A. Perrakis, J. L. Sussman, T. S. Walter, J. Wilson and A. Messerschmidt

Tris(*N,N*-dibenzylcarbamato- κ^2 S, S')bismuth(III)

Tris(*N,N*-dibenzylcarbamato- κ^2 S, S')bismuth(III)

Acta Cryst. (2006). E62, m2552–m2554 [doi.org/10.1107/S1600536806036488]



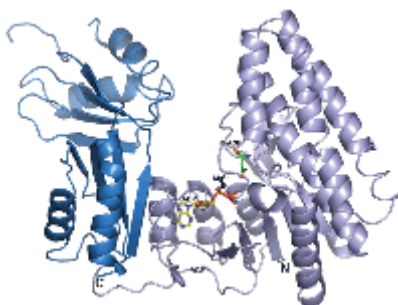
There has recently been increasing interest in bismuth(III) coordination chemistry, particularly in the light of the role of bismuth compounds in ^{212}Bi isotope therapy in cancer research and the use of bismuth complexes in the treatment of peptic ulcers. In particular, the interaction of bismuth(III) salts with chelating dithiocarbamate ligands has been actively studied. In view of the above we report here the synthesis and structure of the title compound, $\text{Bi}(\text{S}_2\text{CNBz}_2)_3$. The coordination polyhedron in the title compound, $[\text{Bi}(\text{C}_{15}\text{H}_{14}\text{NS}_2)_3]$ or $[\text{Bi}\{\text{S}_2\text{CN}(\text{C}_7\text{H}_7)_2\}_3]$, is a distorted trigonal antiprism, with three strong (2.664–2.731 Å) and three weak (2.904–2.965 Å) Bi–S bonds.

F. Li, H.-D. Yin, J. Zhai and D.-Q. Wang

IUCR JOURNALS NEWS

The initial step in the archaeal aspartate biosynthetic pathway catalyzed by a monofunctional aspartokinase

Acta Cryst. (2006). F62, 962-966 [doi.org/10.1107/S1744309106038279]



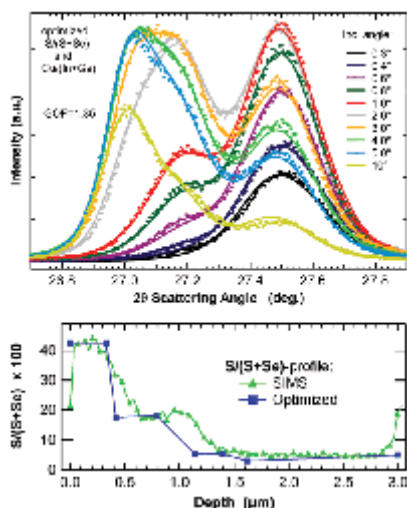
The active site of *M. jannaschii* aspartokinase in a deep cleft formed between the C-terminal ACT regulatory domains (dark blue) and the N-terminal catalytic domain (light blue) within each subunit of the tetrameric enzyme.

The enzyme aspartokinase catalyzes the commitment step to amino acid biosynthesis in the aspartate pathway. The first structure of a microbial aspartokinase, isolated from *Methanococcus jannaschii*, has been determined in the presence of the amino acid substrate, Aspartic acid, and the nucleotide product, MgADP. The enzyme assembles into a dimer of dimers both in the crystal and in solution. The active site groups responsible for substrate binding have been identified, and roles have been proposed for putative catalytic groups.

C.R. Faehnle, X. Liu, A. Pavlovsky and R.E. Viola

Compositional depth profiling of polycrystalline thin films by grazing-incidence X-ray diffraction

J. Appl. Cryst. (2006). 39, 683–696 [doi.org/10.1107/S002188980601987X]



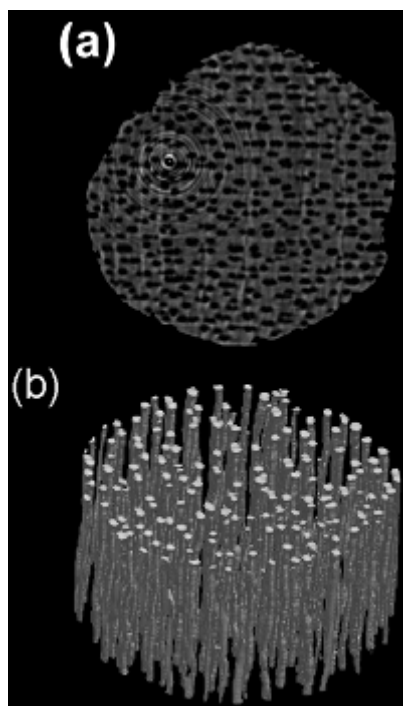
(Top) Measured (dots) and simulated (solid lines) diffraction profiles of the 112 reflection of a $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ thin film; (bottom) Corresponding optimized $\text{S}/(\text{S}+\text{Se})$ depth profile in comparison to a profile obtained by secondary ion mass spectroscopy (SIMS).

A novel pattern matching method for compositional depth profiling of polycrystalline thin films using grazing incidence X-ray diffraction (GIXRD) is proposed. A layer absorption model permits generation of GIXRD patterns on the basis of instrument function, compositional depth profiles and absorption characteristics. In contrast to other methods the modelling approach exploits the information stored in the shape evolution of the peak profile as a function of incidence angle. As an example the Cu and S depth gradients in a 2 μm thick $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ thin film are accurately refined.

I.M. Kötschau and H.W. Schock

Fast tomography using quasi-monochromatic undulator radiation

J. Synchrotron Rad. (2006). **13**, 403–407 [doi.org/10.1107/S0909049506023466]



Reconstructed cross section and three-dimensional structure of a wood stick whose diameter was about 3.1 mm. (a) Cross section. (b) Three-dimensional reconstruction by volume rendering. The area with low density (air) is visualized.

An ultra-fast X-ray CT system was developed at the helical undulator beamline BL40XU in SPring-8. Fast X-ray CT enables us to obtain 4-dimensional information including time resolving ability. This is an important technology for all kinds of sciences. The minimum measurement time was 10 s for 312 projections with a spatial resolution of around 10 μm . The shortest interval between each measurement was about 3 min. The figure shows a CT image of a toothpick obtained with the system in 15 s.

K. Uesugi, T. Sera and N. Yagi

BOOK REVIEW

International Tables for Crystallography Volume G: Definition and exchange of crystallographic data

International Tables for Crystallography
Volume G: Definition and exchange of crystallographic data

Sydney Hall and Brian McMahon, Editors

Published for the IUCr by Springer, 2005

ISBN 1-4020-3138-6, 594 + xii pages

This volume of *International Tables* must be aimed primarily at crystallographic programmers and people looking after the maintenance and distribution of crystallographic data. The sections on the Molecular Information File (MIF) may be of interest to practical crystallographers wishing to save their noncrystallographic information in a digital format closely related to the ubiquitous CIF format, and the final part lists tools to help in the preparation of files for deposition or publication.

Much of the information it contains is available online from the IUCr website. The decision to publish a printed version reaffirms that while digital versions of texts are convenient for keyword searching and occasional reference, current hardware is nowhere near fast enough and current monitors are nowhere near big enough to permit effective browsing and research studies.

Part 1, a Historical Introduction, is more than just a history; it also provides an explanation for why the current crystallographic information files have a syntax that at first sight seems overcomplicated. It shows the care and insight that went into designing and then revising the data dictionaries, which, in effect, are an ordered mechanism for representing almost all crystallographic data. The final section, the relationship between CIF and XML, shows that (fortunately) these two concepts have sufficient in common to make data transfer from one system to the other relatively simple.

Part 2, Concepts and Specifications, develops the ideas introduced in Part 1, and is probably the key section for programmers to study. Section 2.1.3.1, which describes the formal definitions of <blank> (ASCII 32, 11 and 9), <terminate> (ASCII 10, 12 and 13) and <wspace> and their association with the mark-up characters ', " and ; to define text strings, will be important to programmers, as will the portability and archival issues described in Section 2.2.4. For example, to be fully forward compliant, programmers writing codes to read CIF files will need to process text lines consisting of up to 2048 characters (as opposed to the original definition of 80 characters). The specification of the Crystallographic Binary File (CBF/imgCIF) describes how figures and drawings, together with diffraction images, can be included into CIF-like files. Section 2.5 (core CIF dictionary definition language, DDL1) and Section 2.6 (relational dictionary definition language, DDL2) explain the concepts behind the many data items described later in the volume.

Part 3, CIF Data Definition and Classification, is 130 pages of carefully written explanations of the practical issues in defining data items, covering the core data, powder diffraction, modulated and composite structures, macromolecular data, image data and symmetry data. The CIF concept enables individuals or laboratories to define and register data items for their own use, and include them in data files. These will be read but ignored by a properly compliant CIF-reading program. However, there are very many data items that will be in very widespread use, and which should thus have carefully thought

out published definitions. The IUCr Committee for the Maintenance of the CIF Standard (COMCIFS) has the task of producing and maintaining these fundamental definitions.

Part 4, Data Dictionaries, occupies almost half the volume, and gives the current definitions of all data items to be found in the various data dictionaries. This is the section that most benefits from having an electronic version available online, as that can be quickly searched without one having to know the exact data name.

Finally, Part 5, Applications, provides advice for programmers and CIF users. It details libraries of useful CIF facilities that can be built into other applications, and also complete applications that can be downloaded or accessed, mostly free of charge, for editing, validating and manipulating CIF. It is the section that will most rapidly become out of date. The volume also includes a CD containing most of the tabular material, software libraries and end-user applications.

The CIF format has more or less become the international standard for the deposition and publication of crystallographic results, and increasingly application programs will accept CIF as an input format. Most practising structure analysts will expect their normal software systems to create the bulk of a CIF for each structure. However, most CIFs will require some additional manual editing — increasingly so as journals become willing to accept whole papers in CIF format.

International Tables Volume G will be an invaluable reference to help ensure that edits are compliant, and may also encourage crystallographers to store other information along with the minimal crystallographic details. Every active crystallography group should have a copy of this book.

Reviewed by David Watkin

Chemical Crystallography Laboratory, U. of Oxford, UK

AWARDS AND PRIZES

IUCr wins prestigious international award for publishing innovation



The IUCr has won the 2006 Award for Publishing Innovation of the Association of Learned and Professional Society Publishers (ALPSP).

The Award, for Data Exchange, Quality Assurance and Integrated Data Publication (CIF and *checkCIF*), recognizes the involvement of the IUCr in the development of the Crystallographic Information Framework and its applications, for example

- standard data definitions for crystallographic information archive and interchange
- submission format for structure report articles in crystallographic journals
- standard format for depositing supplementary structural data accompanying publications
- automated checking of the integrity and self-consistency of crystal structure models (the web *checkCIF* service)
- use of *checkCIF* as a peer review tool
- dissemination of crystal structural models in online publications and automated visualization.



Brian McMahon (left), IUCr R&D Officer, receives the award from Bernard Donovan, ALPSP President, at the Association's annual dinner on 14 September 2006 at the Armourers' Hall in London, UK.

The judges felt that in developing CIF and *checkCIF*, the IUCr has established an important example of data quality assurance with potential applications in other scientific, medical and indeed social sciences publishing.

The crystallographic information file (CIF) and associated data dictionaries allow the seamless transfer of information from experimental apparatus, through computation analysis, to database deposition and publication. CIF also allows the definition of quality standards for data deposition and publication and the deployment of mechanisms for checking compliance with such standards, via the *checkCIF* web-accessible service. The main features of the standard are its well-defined machine-readable syntax, large collection of individually defined data names and the formalism that allows automatic validation of certain attributes of data. The standard has been extended to assist with routine aspects of editorial checking and peer review, which can now take place with much increased speed and confidence.

The judges were impressed with the way in which CIF and *checkCIF* are easily accessible and have served to make critical crystallographic data more consistently reliable and accessible at all stages of the information chain, from authors, reviewers and editors through to readers and researchers. In doing so, the system takes away the donkey-work from ensuring that the results of scientific research are trustworthy without detracting from the value of human judgement in the research and publication process.

The development and maintenance of CIF and *checkCIF* is sponsored by several publishers but it is freely accessible to all. The IUCr already works closely with other related structural science communities and is looking to extend this cooperation.

"The IUCr is honoured by the 2006 ALPSP Award for Publishing Innovation," said Peter Strickland, Managing Editor, IUCr Publications. "The award recognises the hard work and dedication of our publishing staff and academic collaborators, and the role that learned societies can play in introducing novel and valuable contributions to scientific information exchange. The Crystallographic Information Framework owes much to the special nature of crystallography and its relatively compact community of practitioners but we hope that this award will encourage other scientific disciplines to follow similar approaches to integrating research data and literature, and to extending the tradition of peer review more deeply into the supporting data."

SPECIAL REPORT

Crystallography in Singapore

An overview



Swami begins with his experience when he decided to move to Singapore. “In 1998, the most important doubt for my then 8 year old son was whether pizza would be available there. With my knowledge of geography and his level of comprehension I convinced him that Singapore is just an extension of California but there is a big ocean in-between. I even managed to make him believe that there would be bus service between Singapore and Los Angeles. After moving to Singapore I learned very soon that the kids of my ‘expat’ (a term we use here for foreign workers) colleagues had similar doubts about burritos, sushi, masala dosa and so on”.

Singapore is a small island of about 690 sq. km with a population of ~4 million people. It is essentially a city country with no natural resources, but this has not hampered the country’s growth since its independence from Malaysia in 1965. Within a short span of time Singapore has become a highly developed country with a successful free market economy. Until the beginning of the 1990s Singapore was known mostly for economical shopping. Recently, it has become a choice destination for scientists, especially crystallographers as can be seen from the increase in the number of crystallographers and research areas over the past 10 years.

“Crystallography is very new to Singapore”, according to Lip Lin Koh who returned to Singapore in 1964 from Boston University. He was not aware of any crystallographic research or teaching in Singapore or Malaysia at that time. All three universities (U of Malaya at Kuala Lumpur, U of Malaya at Singapore and Nanyang University, Singapore) had Physics and Chemistry departments, but crystallography was not part of the curriculum. He was the first to introduce crystallography as part of Physical Chemistry. In the mid 1970’s, he was able to obtain a table-top X-ray unit, a Weissenburg camera and a Debye-Scherr camera. These were mainly used for demonstration and simple experiments and projects for senior undergraduate students. The first crystal structure publication from Singapore was: Thianthrene gold (III) chloride (chloroform solvate) at -70 °C. N.W. Alcock, K.P. Ang, K.F. Mok, and S.F. Tan. *Acta Cryst.*, **B34**, 3364 (1978). K.P. Ang was a former head of the chemistry department, National University of Singapore (NUS) and S.F. Tan was an emeritus professor in the same department.

It was only in October 1989 that the first single crystal X-ray diffractometer (a Siemens P3) with a MicroVax computer arrived at the Department of Chemistry, NUS. Koh says, “It was with this instrument that I was able to become a crystallographer again, picking up my skills after 20 years! Luckily, I still remembered my crystallography, thanks to the physical chemistry that I had been teaching and my sabbatical leave in 1987”. The first researchers to actually use the diffractometer were: K.F. Mok (after retirement he moved to Nanyang Technological University (NTU)), and W.L. Kwik (deceased), followed by Y. Lam and Y. Xu (Koh’s postdoc from 1992 to 1995). Xu left for the National Institute of Education (NIE) in 1996 to start her own X-ray crystallography lab equipped with a P4 diffractometer. The current service facility at the Department of Chemistry, NUS was established in 1997 when the first Siemens SMART 1000 CCD diffractometer arrived, and Jagadeese J. Vittal, an experienced chemical crystallographer from Canada, joined the faculty. Now more than 20 faculty members from the department of chemistry and

their research groups routinely use this facility.



Geok Kheng Tan

Geok Kheng Tan, who maintained the P3 in the earlier days, is now taking care of four diffractometers. She is likely to hold a record for collecting and solving at least 5000 newly synthesized small molecule structures in Singapore. After training in Germany and Japan, George Tang (now General Manager, Bruker, Singapore) returned to Singapore as a salesman for Siemens and sold the first diffractometer in Singapore. He also confirms that an old Siemens powder XRD system was installed in Robertson Research, a commercial geological lab, in 1989.

Macromolecular crystallography in Singapore started in 1997 after Prasanna Kolatkar arrived. Also Nam-Hai Chua, one of the founding professors of the Institute of Molecular and Cell Biology (IMCB, 1987) established the Institute of Molecular Agrobiolgy in 1995 (now called Temasek Lifescience Laboratories, TLL) and recruited some of the early birds in 1998. Subsequently, the Singapore government has undertaken a strong commitment to promote Singapore as a biotechnology power-house in this region. Through the National Science and Technology Board, which is now known as the Agency for Science, Technology and Research (A*STAR), the government has established more research institutes. In addition, NTU established its School of Biological Sciences and recruited several crystallographers. In summary, the two universities, NUS and NTU (with their appropriate departments or schools), and several research institutes, like IMCB, Genome Institute of Singapore (GIS) and TLL, are now very actively involved in macromolecular crystallographic research.

Chemical crystallography

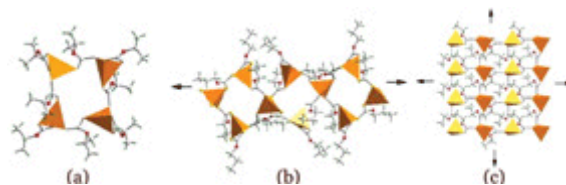


Fig. 2.1. The structures of $\text{Zn}(\text{S}_2\text{COR})_2$ where R = iso-propyl (a), n-propyl (b) and ethyl (c) groups. Edward R.T. Tiekink had a brief stint at NUS (2001-04) before joining the University of Texas at San Antonio in the Fall of 2005. While at NUS his research interests revolved around chemical crystallography with an emphasis on main group element chemistry, the development of metal-based drugs for the treatment of cancer, rheumatoid arthritis and tropical diseases and new molecular materials. His work on steric control of supramolecular aggregation is nicely illustrated in a series of three binary zinc xanthate structures as shown in Fig. 2.1.

Jagadeese J. Vittal confessed that he was really afraid of symmetry and space groups when he was a graduate student. During his postdoc at the University of Western Ontario he was encouraged to take the crystallographic course offered in the Chemistry Department. He fondly recalls that his mentor in crystallography, Nicholas Payne, “was a dedicated crystallographer who really enjoyed teaching crystallography. He patiently taught me to be a well-rounded crystallographer”. Later Vittal was a service crystallographer in the same department before he accepted a position at NUS in 1997. The Siemens CCD diffractometer, installed in the Department of Chemistry at NUS in 1997 was not only the first one in Singapore but also in that region and it was one of the reasons Vittal moved to Singapore.

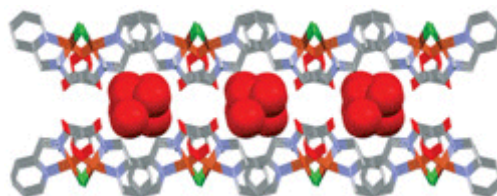


Fig. 2.2. The water chains formed in a coordination polymeric host lattice $[\text{Cu}(\text{pgly})\text{Cl}] \cdot \text{H}_2\text{O}$. The hydrogen atoms are not shown.

Being a crystallographer by profession and synthetic inorganic chemist by training, he initiated a research program in crystal engineering and chemistry of metal thiocarboxylates. His experience in crystallography helped him to venture into nanocrystals. He is currently interested in the supramolecular transformation of structures, aligning double bonds in coordination polymers in the solidstate and water clusters. The structure of water chains hosted by an inorganic crystal lattice from his work is illustrated Fig. 2.2.

Yulin Lam, from the Department of Chemistry, NUS, is one of a very few Singaporeans trained and currently practicing chemical crystallography in Singapore. She received her PhD from NUS (Supervisor: Hsing Hua Huang) in the area of conformational analysis. She was a Research Fellow at the Scripps Research Institute and the Institute of Molecular and Cell Biology in Singapore before joining NUS. Her research interest includes combinatorial chemistry, structure-based and pharmacophore-based drug design and conformational analysis.

Siau Gek Ang is one of the chemistry faculty members who is interested in the application of spectroscopic techniques and X-ray diffraction methods. Her research interests include bioactive compounds from Chinese herbs and the organometallic chemistry of osmium and ruthenium. Currently she is Registrar of NUS.

Weng Kee Leong is using single crystal X-ray crystallographic techniques to elucidate the solid-state structures of newly synthesized heteronuclear and intermetallic clusters, nanomaterials and heterogeneous, and homogeneous catalysts.

Feng Xu, a new member of the chemistry faculty of NUS, is interested in both chemical crystallography and macromolecular chemistry. He learned chemical crystallography as a graduate student in the Chinese University of Hong Kong under Tomas C.W. Mak. He worked in macromolecular crystallography at the Wistar Institute, Philadelphia, USA before coming to Singapore in 2005. He is interested in supramolecular chemistry and crystal engineering of hydrogen-bonded molecular solids; design and control of molecular assemblies and packing arrangements to generate crystals with specific properties as new materials and drugs; structural biology of viruses by X-ray crystallography; molecular modeling and electron microscopy; and understanding protein structure and its biological function for pharmaceutical application.



Tim White

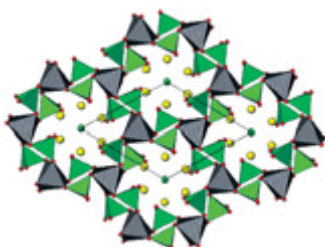


Fig. 2.3. Structure of $\text{Ca}_{10}(\text{AsO}_4)_6\text{F}_2$, svabite (a structural analogue of apatite)

Tim White is at the School of Materials and Engineering, NTU. He is interested in crystallographic investigations of functional ceramics using electrons, X-rays and neutrons, especially materials related to environmental remediation and catalysis. His structure of triclinic $\text{Ca}_{10}(\text{AsO}_4)_6\text{F}_2$ svabite is shown here (Fig. 2.3). He received his PhD from the Australian National University and has had postdoctoral research experience in practically every capital city in Australia, the USA, Germany and Japan. He has been in Singapore for more than a decade beginning with the establishment of the Environmental Technology Institute in 1996. Presently, he is the Director of the Facility for Analysis, Characterization, Testing and Simulation (FACTS) which is the largest multipurpose electron microscopy and X-ray diffraction laboratory serving the crystallographic community in Singapore. Tim says, "Singapore is an unusual, and possibly unique country, in which to build a research group. The support for research is tremendous, but an appreciation of the utility of fundamental scientific investigations such as crystallography is only just developing. Undoubtedly, the many opportunities to create international collaborations are the most invigorating aspects of working in Singapore, and our group has developed strong links with groups in Australia, Europe and the US."

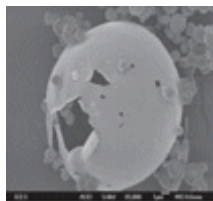
Kum Fun Mok is one of the distinguished crystallographers in Singapore. After retirement from the Department of Chemistry, NUS, he established the X-ray Crystallography unit for the Division of Chemistry and Biological Chemistry, NTU along with his former student Yongxin Li.



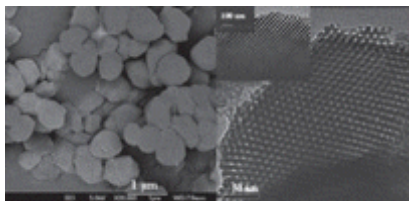
Reginald Tan



a



b



c

Fig. 2.4. (a) The crystalliser system with ATR-FTIR and FBRM monitoring and control. (b) Spray-dried large hollow nano-particulate aggregate of 20 nm silica nano-particles. (c) Monosized nanoporous siliceous submicron excipient particles, synthesized via a novel environmentally benign dry gel conversion route.

Reginald B.H. Tan is the Programme Manager of Crystallization and Particle Science at the Institute of Chemical & Engineering Sciences (ICES). ICES is one of the twelve research institutes of A*STAR. He obtained his PhD in chemical engineering from the University of Cambridge and his research interests include modeling of transport phenomena, crystallization and formulation sciences. He also holds an Associate Professorship in the Department of Chemical & Biomolecular Engineering (ICES) at NUS. At ICES he leads a team of more than 20 scientists and engineers in investigating crystallization and formulation sciences from fundamentals to industrial applications. His team is currently studying the fundamental scientific principles underlying nucleation and crystallization phenomena, with the aim of controlling crystal size, shape, form, purity and formulability. He is also implementing his results for industrial applications with the aid of process analytical technology (PAT). In the area of formulation sciences, Tan's group is actively studying topics in particle formation and design, powder technology and interfacial phenomena related to pharmaceutical and fine chemical applications. He is also investigating novel formulations in potentially valuable areas, including co-crystals and nanoparticle drugs, functional excipients and direct precipitation of stabilized fine particles (see Fig. 2.4). Ning Shan is a Research Fellow at ICES interested in crystal engineering, crystallization and molecular modeling. He did his Ph.D. at Cambridge, UK and was a visiting engineer at the Massachusetts Institute of Technology in 2004-2005.



Chris Boothroyd

Chris Boothroyd is a Principal Scientist in the Institute of Materials Research and Engineering (IMRE, one of the institutes of A*STAR) where he is in charge of the electron microscopes. He has 24 years of experience in transmission and scanning electron microscopy including energy loss spectroscopy (EELS), energy filtered microscopy (EFTEM) and high resolution electron microscopy (HREM). In the past he worked in the electron microscopy group at the Department of Materials Science and Metallurgy, Cambridge, where his research covered a wide variety of topics related to electron microscopy. Currently he is interested in the quantitative measurements of contrast in HREM and its comparison with image simulations. His recent work has been on measurement of phonon scattering and its contribution to HREM using convergent beam and holographic methods. Apart from hardcore single crystal diffraction studies, several scientists are working on chemical vapor deposition, surface science problems such as self-assembly, reactivity of molecules, functionalizing metal surfaces, etc. Also, experimental techniques such as low energy electron diffraction (LEED), high resolution electron energy loss spectroscopy (HREELS), X-ray photoelectron spectroscopy (XPS), ultra-violet photoelectron spectroscopy (UPS) and Auger electron spectroscopy (AES) are also being used extensively.

Nobel Laureate Robert Huber is a visiting faculty member at the Department of Chemistry, NUS and teaches an MSc Industrial Chemistry course, jointly offered by NUS and the Technical University of Munich. He is a familiar face at the NUS campus.

Macromolecular crystallography



Prasanna Kolatkar (extreme right) with his group members

The density of charged amino acids per unit surface area is ... oops, we are lost. Yes, now we remember. When you come to macromolecular crystallography, you will be surprised to know that the density of protein crystallographers in Singapore is significant! There are 9 protein crystallography labs on this tiny

island. The first protein crystallographer to land in Singapore in 1997 was Prasanna Kolatkar (popularly known as PK), from Michael Rossmann's lab. He did his Ph.D. at University of Texas at Austin and a Postdoc at Purdue. He is working on the structural Biology of transcription factors and proteins involved in stem cell and cancer biology and analysis of protein-protein interactions. He is now a senior investigator at the Genome Institute of Singapore, one of the A*STAR research institutes.



Fig. 3.1. Structure of five mushroom protein derived from Golden needle mushroom.

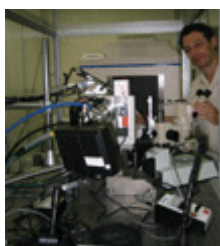
PK says, "My time in Singapore has been well spent as I have had access to funding at a reasonable level to do good science. In addition I have been able to recruit many talented people from around the world including Norway, Germany, India and China as well as the US over the years. In addition a growing pool of Singaporean talent has helped to fill manpower needs in the lab. We have been able to determine the structures of several interesting proteins including the five mushroom protein (Fig. 3.1). We have also carried out structural bioinformatics related work dealing with protein-protein interactions and relationships of domains. I would like to see a much greater output of quality structures and interesting findings in the future. I also am hoping to better integrate my informatics and wet-lab portions of the lab to focus on transcription factors".



Swami dressed like Indian Nobel Laureate Sir. C.V. Raman

The next to join the club in 1998 were Kunchithapadam Swaminathan (Swami) from the Wistar Institute, Philadelphia and Terje Dokland (now at the University of Alabama, Birmingham) from Purdue.

Swami says, "My first day in Singapore was laced with childhood memories. Interestingly, in third grade (1969) in my village school, a friend's grandfather returned to our village after a trip to Singapore. In fact, we used to call him 'the great man who traveled in a ship'. He presented me with a pencil with a small eraser attached at the end. Even today, this pencil is one of my most unforgettable surprises. After that I saw Singapore in several Indian films. However, I never had a chance to come here".



Julien Lescar behind his instrument.

Swami did his Ph.D. at the Indian Institute of Technology, Mumbai, India (1989) and post-doctoral research at Penn (1989-95) and the Wistar Institute (1995-97). Currently he heads two labs, one at the Institute of Molecular and Cell Biology and the other at the Department of Biological Sciences, National University of Singapore. "In one of the Scientific Advisory Board meetings, Nobel Laureate Sydney

Brenner (who also has a lab at IMCB) joked with me that I am a bigamist. I just replied that I enjoy it! If I have to comment about science in Singapore, the efforts by A*Star, NUS and NTU to promote quality research and publication are wonderful. Funding is sumptuous. There is no problem for facilities, resources and freedom. At the same time the level of competition is challenging.”

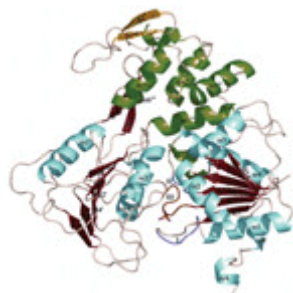


Fig. 3.2. A view of the dengue ns3 helicase catalytic domain structure

Haiwei Song is another protein crystallographer at IMCB who came from Oxford University in June 2001. Julien Lescar came next. He was originally trained as a Physicist (University Paris XI, Orsay, France) but became gradually more interested in macromolecular recognition in the immune system through the study of antigen-antibody complexes during his Ph.D. and a Postdoc at the Immunology Department of the Pasteur Institute in Paris (1990-1996). In January 1997, he moved to the European Synchrotron Facility in Grenoble, where he took an active part in the development of the ID2 High Brilliance Bio-Crystallography Beamline, maintained by the European Molecular Biology Laboratory (EMBL). In September 1999, he was a research scientist at the University Joseph Fourier in Grenoble where he got involved in several studies on Protein-Carbohydrate interactions. In January 2002, he came to Singapore to take part in the launching of a new School of Biological Sciences at NTU. A schematic view of the dengue ns3 helicase catalytic domain structure from his lab is shown in Fig. 3.2.

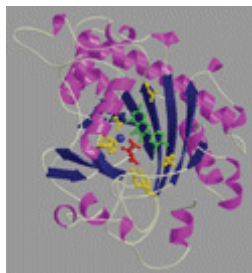


Fig. 3.3. Structure of anthocyanidin synthase

Rupert C. Wilmouth is also a faculty member of the School of Biological Sciences, NTU. He got his Ph.D. and post-doctoral experience at University of Oxford. His field of research includes mechanistic crystallography, proteases, helicases and kinases. On the research experience in Singapore, Rupert says, “Very good: excellent new buildings, superb quality and quantity of research equipment, good level of grant funding. Main downside so far has been difficulty in recruiting researchers. My only wish list is a synchrotron suitable for protein crystallography in Singapore”! His structure of anthocyanidin synthase from *Arabidopsis thaliana* is shown in Fig. 3.3.



J. Sivaraman (inset) with his team.

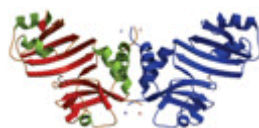


Fig. 3.4. Crystal structure of RluF

Our next player J. Sivaraman, who moved to Singapore in July 2003, did his PhD (1995) at Anna University, India and his post doctoral research (1995-2003) at the Biotechnology Research Institute, National Research Council of Canada, Montreal. "Singapore is an exciting place to do research because science has been targeted as a key to the country's future development. This is especially true in the life sciences area, where many research opportunities are available at institutes, universities, and companies. In our lab we are focusing on the crystal structure and catalytic mechanism of several cysteine proteases of the papain superfamily, ribosomal RNA modifying enzymes and enzymes involved in carbohydrate metabolism". His recent crystal structure of RluF is shown in fig. 3.4.



Bob Robinson & his team.

Bob Robinson (who is carrying his lab members on his head in the figure in the photograph) is from Lancashire, England and completed his B.Sc. in chemistry at King's College, London University and an M.Sc. in the same subject at the University of British Columbia, Vancouver. After working at Regeneron Pharmaceuticals in New York, he undertook a D.Phil at Oxford University specializing in protein crystallography and then did a postdoc at the Salk Institute, San Diego. Bob started the Actin Structure Laboratory at Uppsala University, Sweden. His group moved to IMCB in the spring of 2005 where he is an Associate Professor.

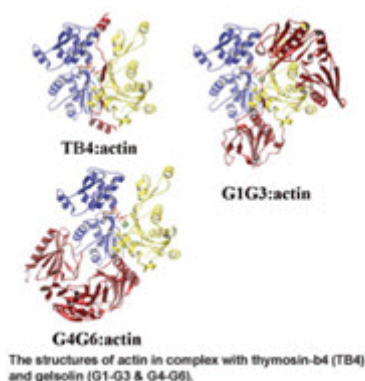
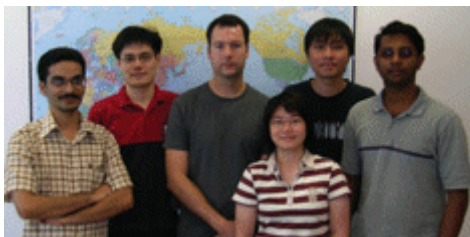


Fig. 3.5. Actin polymerization machinery proteins

"IMCB provides a stimulating environment for science. I made the jump from a granting system to a fully funded Institute. In this system scientists can dedicate their time to doing science, rather than hypothesizing about what they would like to be doing, and target questions without excessive limitations of time and resources. We are pretty much only limited by our own abilities and imaginations."

Bob's main interest is in understanding the mechanisms behind cell movement. The Lab focuses on actin polymerization machinery (related structures above), which provides the force during cell locomotion.

“We use protein crystallography to determine the shape of key molecular complexes that regulate the spatial and temporal patterning of actin assembly and disassembly. In the long term we would like to design drugs to interfere with these processes, with the aim of stopping pathogens and cancer cells from invading tissues or to speed up the recruitment of repair cells to wound sites.”



Curt Davey (third from left) with his research team.

Curt Alexander Davey [Ph.D., Univ. of Miami School of Medicine, USA (1996), Postdoc, Univ. of Miami, USA (1996-1997), staff scientist postdoc, ETH-Zurich, Switzerland (1998-2003)] is now an Assistant Professor, Division of Structural & Computational Biology, School of Biological Sciences, NTU. “My lab is interested in the molecular and atomic details of how the expression of genetic information is regulated. Our main focus is on structural characterization of large DNA-protein assemblies, such as the nucleosome core particle of chromatin, using primarily X-ray crystallography. In particular, we are studying the relationship between DNA sequence, protein binding, and the resulting DNA conformation, and how this protein-bound DNA conformation influences association of small molecules or additional protein factors.

In Singapore, research in the biological sciences is on the rise. The current funding atmosphere holds special promise for investigators who are embarking on novel research avenues or engaging in unique interdisciplinary ventures. For the hard-core X-ray crystallographer, the only major item to wish for would be to have our own macromolecular synchrotron facility!”

The latest addition to our club is Adam Yuan (another bigamist) from Memorial Sloan Kettering Cancer Center, New York. He will have a joint appointment with Temasek Life Science Laboratory and the Department of Biological Sciences, National University of Singapore.

Singapore Synchrotron Light Source (SSLS)



SSLS Director Herbert O. Moser

Don't you think the wish of all crystallographers for a synchrotron in Singapore should be fulfilled? Yes, Singapore now has its own synchrotron. According to Herbert O. Moser, Director of SSLS, “Singapore is a special place for synchrotron radiation. Due to the strong concentration of high-tech industries and the high level of scientific research and education there is a huge potential for synchrotron radiation applications. The mission of SSLS is to bring synchrotron radiation into industrial, institutional, and academic daily life in order to add value to the wealth-creating process”.



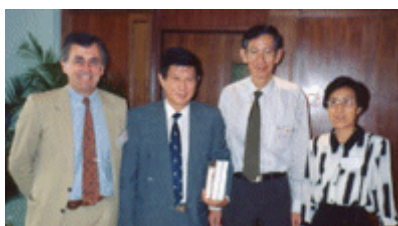
SSLS building on the campus of the National University of Singapore.

The Singapore Synchrotron Light Source (SSLS, <http://ssls.nus.edu.sg>) is a university-level research institute at NUS. It is dedicated to generating and exploiting synchrotron radiation for research and development purposes and provides services for customers including research institutions, industry and institutions of public interest. At present, synchrotron radiation is produced by a compact 700 MeV electron storage ring with two 4.5 T superconducting dipoles. It covers a spectral range of 7 orders of magnitude from hard X-rays to the far infrared. Five beamlines and experimental stations are in operation comprising a micro/nano-manufacturing facility (LiMiNT), a phase contrast imaging and tomography beamline (PCIT), a soft X-ray facility for surface, interface, and nanostructure science (SINS), a hard X-ray facility for diffraction, absorption spectroscopy and fluorescence (XDD, X-ray demonstration and development) and an infrared spectro/microscopy facility (ISMI). A further beamline for electron beam diagnostics will be ready in 2006. This portfolio of experimental facilities makes SSLS rather attractive for a wide variety of research disciplines including biomedical engineering, catalysis, data storage, environmental science and engineering, life sciences, materials science and engineering, micro/nanotechnology and semiconductor manufacturing.

The XDD beamline was designed for general-purpose diffractometry including high-resolution diffractometry, powder diffractometry, reflectometry, and topography. It also features XAFS (X-ray absorption fine structure). With high-resolution diffractometry, precise structural parameters, minute strain status, composition, thickness, surface/interface roughness and texture/stress analysis for crystalline materials can be obtained. Powder diffractometry makes possible crystal structure determination and refinement, phase identification both in quality and quantity, precise lattice-parameter determination, measurement of crystal grain size & texture/stress analyses. With grazing-incidence-diffraction, reflectometry and diffuse scattering, information on surface and interface structure ordering, as well as surface phase identification/transition can be obtained. XAFS can offer information on neighboring coordination and valence status in a complex, particularly for non-crystalline materials.

SSLS has proposed to disentangle the methods currently combined in XDD and to build dedicated beamlines for powder diffraction, for long-wavelength macromolecular structure determination enabling phasing from phosphorus up (2.149 keV) and for X-ray absorption fine structure spectroscopy, all of them serving research institutes, universities, and industry, locally as well as regionally. They are also slowly expanding in other areas like XAFS, XANES (X-ray absorption near edge structure) and reflectometry.

Conferences, meetings and workshops



From L to R. Syd Hall, Peter Huang, L.L. Koh and Yu Wang at AsCA'92.

Asian Crystallographic Association Meeting (AsCA'92): The Inaugural AsCA Conference was held in Singapore, in November 1992. The Crystallographic Society of Japan and the Society of Crystallographers in Australia and New Zealand supported this by holding their annual meetings at AsCA'92. Syd Hall of Western Australia was the conference chairman and Lip Lin Koh chaired the local organizing committee. The then President of the IUCr, Andre Authier, attended the meeting. The total registration was 320 from more than 20 countries with 260 full participants and 60 students, excluding 30 accompanying persons. The scientific program consisted of 16 oral sessions with 73 papers and 22 poster topics with 190 papers.

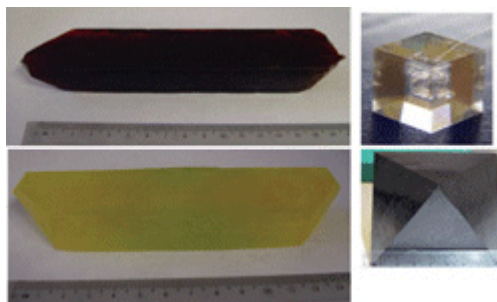


Fig. 4.1. Some of the crystals grown by high school students in the crystal growing challenge Singapore National Crystal Growing Challenge:

The crystal growing challenge has been very popular among students from secondary schools, junior colleges and polytechnics in Singapore. In this challenge the students have an opportunity to show their creativity and learn about the science and art of growing crystals. The crystal growing challenge is designed to reveal the importance of the technique, to show that science can be fun, and to get students interested and involved in scientific activities at a young age. NUS and the Singapore National Institute of Chemistry organize this event which was initiated by J.J. Vittal in 1997 and conducted with the support of the Department of Chemistry at NUS. Since 2000 it is conducted once in two years. The 6th challenge was conducted in September 2004 with a record number of participants (168 entries from 68 educational institutions). The number of entries has doubled since the first challenge. Each year we are challenging these young minds with new innovative crystal growing challenges such as crystals inside crystals, the longest single crystal, cubic or tetrahedral shaped NaClO_3 , bluish-green $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ but not greenish $\text{NiSO}_4 \cdot 7\text{H}_2\text{O}$. The students have responded well to these challenges. This has been generously sponsored by various agencies from time to time but George Tang of Bruker Singapore has been a constant supporter of this event ever since it started. The winning crystals are kept in display cabinets decorating the chemistry department for two years until the next challenge. Details of the current challenge (September 2006) are available at the website: www.chemistry.nus.edu.sg/ncgc1.htm.



(Left to Right) R.J. Puddephatt, Richard Robson and Stuart R. Batten at the ICMAT 2003 Meeting.



Organizers J.J. Vittal (left) and S. Valiyaveetil (right) with Gautam R. Desiraju at the ICMAT 2003 meeting. Edward Tiekink, another organizer, is missing from this photograph.

New Materials by Crystal Engineering Design Symposium: This symposium, which was one of the symposia of the International Conference on Materials for Applied Technologies (ICMAT 2003), was organized by J.J. Vittal, Edward R.T. Tiekink and Suresh Valiyaveetil during December, 2003. Covered topics included prediction of crystal structures, polymorphism, metal coordination polymers, and magnetic and optoelectronic materials. A highlight of the meeting was a session to honor Richard Robson for his contributions to crystal engineering. Over 70 registered delegates from 17 countries presented 44 oral presentations in 11 scientific sessions over 5 days and featured 3 poster sessions.



Speakers at the 2004 conference



A model building session at the workshop

International Conference of Structural Biology: The Department of Biological Sciences hosted three International Structural Biology Conferences (2000, 2002 and 2004). The participants of the 2004 conference included Jack Johnson, Susan Taylor and Roger Tsien. Very importantly, in the 2004 conference they conducted a 3 day crystallography workshop that covered all aspects of crystallography. The workshop was free and about 50 graduate students from countries like India, China, and Malaysia attended. The Department of Biological Sciences is now gearing up for the 4th conference in December 2006.



Workshop participants at the 2004 International Structure Biology Conference

By now you might have realized that most Singaporean crystallographers are active, enthusiastic and striving hard to achieve their best. Each time you see the name Singapore, we hope you will remember us. Next time you cross Singapore or plan a wonderful vacation here, along with your rush to enjoy curried fish-heads or pepper crabs, please plan to give a seminar at NUS, NTU or any one of the research institutes of A*STAR!

Kunchithapadam Swaminathan and Jagadese J. Vittal

Singapore's leading crystallographer



Lip Lin Koh

Lip Lin Koh is the most distinguished X-ray crystallographer in Singapore. He received his B.Sc. degree from Nanyang University in 1959 and Ph.D. degree from Boston University in 1964 on the crystal structure of tris(p-aminophenyl)carbonium perchlorate which was published in *Acta Cryst.*, **B27**, 1405-13 (1971). He taught at in the Department of Chemistry at Nanyang University (1964-79) and at NUS (1980-96). He was the first Dean of Science at NUS (1981- 85), and had previously served as Head of the Department of Chemistry and Dean of Science at Nanyang University, before the merger of Nanyang

University and University of Singapore. Apart from his enduring contributions to the university, he also provided service to the public. From 1979 to 1996, he was an elected Member of Parliament of Singapore, playing his part in national policies. He also served the University as a member of the Council. He is currently the president of the Singapore Association for the Advancement of Science. After his retirement from the Department of Chemistry, he was engaged as a part-time research fellow at CE Resources Pte Ltd, an NUS spin-off company.

He rejoined the Department as an Adjunct Senior Research Fellow in 1992, offering selfless guidance to staff and students on solving crystal structures. He was the first Singaporean to serve as a co-editor of the scientific journal *Acta Crystallographica* (during the period 1994-97). He organized the first AsCA Meeting in 1992. He has been helping the Singapore National Crystal Growing Challenge organizers in selecting the winners.

MEETING REPORT

ACA 2006

Honolulu, HI, USA, July 22-26, 2006

The American Crystallographic Association held its annual meeting in a lovely place this year, Honolulu, Hawaii. Thanks to the exciting scientific program planned by Program Chair Judith Kelly, along with members of the eProgram Committee: Simon Billinge, Bryan Chakoumakos, Lachlan Cranswick, Aina Cohen, Chad Haynes, Charles Kissinger, Thomas Koetzle, Jeanette Krause, Paul Langan, Craig Ogata, Allen Oliver and Volker S. Urban; the hard work of Local Chairs Charlie Simmons and Karl Seff, and (probably) in some part due to the spectacular venue overlooking the Pacific, the meeting was among the largest the ACA has ever held, almost 1000 attendees. It was by far the most international of our meetings: 25% were non-US crystallographers and 10% of the abstracts were from Pacific Rim countries. Some of the highlights of the meeting, as excerpted from the Fall ACA Reflexions, follow. Regrettably the selection is far from comprehensive, and probably not even representative. *Connie Chidester*



ACA Vice President Alan Pinkerton with Howard Einsphar and Frank Fronczak.

ACA *Transactions* are always published, and the 2006 Transactions Symposium topic was “The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecule.” The first session, devoted to discussion of the present status and future prospects for neutron crystallography, was organized and reported by Tom Koetzle and Ray Teller. Facilities at the ISIS facility (UK) and the Spallation Neutron Source at J-PARC (Japan) were reviewed; both are developing instruments optimized for macromolecules: a new BIX-P1 diffractometer at J-PARC, and LMX, a Large-Molecule Diffractometer for Supramolecular Chemistry and Biological Structure, which will reside on the new cold neutron target station (TS2) that is under construction at ISIS. Facilities in the US include the Argonne Intense Pulsed Neutron Source, the Los Alamos Neutron Science Center, (the Protein Crystallography Station (PCS) at Los Alamos is currently the only instrument in the U.S. dedicated to neutron protein crystallography). The accelerator-based Oak Ridge Spallation Neutron Source in Tennessee was completed last spring, and when ramped up to full power, the SNS will provide the most intense pulsed neutron beams in the world.



Paul Langan and Alberto Podjarny organized the second session of the Symposium; their report emphasized how advances in instrumentation and sample preparation methods are pushing the limits of macromolecular structure determination. Wolfram Saenger's studies of cyclodextrins showed the extraordinary power of neutrons to elucidate details of hydrogen bonding. The power of neutron diffraction for visualizing hydrogens in enzymes was obvious in the structures presented by Alberto Podjarny (aldose reductase), Gerry Bunick (xylose isomerase), and Chris Delwis (dihydrofolate reductase). These structures are some of the largest ever studied by neutron crystallography and

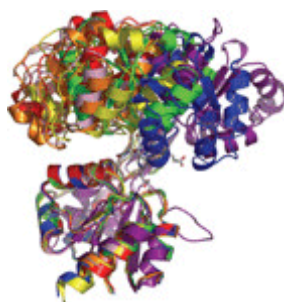
remarkably were achieved by using crystals as small as 0.15mm. Dean Myles described the MACromolecular Neutron Diffraction beam line, MANDI, which is planned for the next generation spallation neutron source at ORNL. New beam lines on next generation sources, in combination with deuteration support laboratories being developed at Los Alamos, Oak Ridge and Grenoble, will continue to push neutron macromolecular crystallography towards smaller samples and larger and more complex problems.



The 2006 Martin J. Buerger Award was presented to Helen Berman by ACA President Bob Bau at the Symposium organized in her honor. The award recognized her lifetime work in the pioneering development of information services for the global research community of macromolecular researchers. She played an influential role in the conception and early development of the Protein Data Bank and pioneered new methodologies in the creation and maintenance of the Nucleic Acid Database. Under her leadership, the Research Collaboratory for Structural Bioinformatics (RCSB) assumed responsibility for the PDB in 1999. Helen is a Board of Governors Prof. of Chem. and Chemical Biol. at Rutgers. Helen opened the session by taking the audience on a “Personal Journey Through Crystallographic Space”. The remaining speakers had all interacted with Helen at some point during her career.



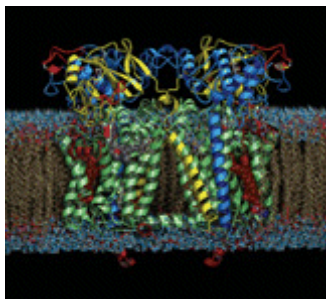
The Bertran Eugene Warren Award for 2006 was presented by Bob Bau to Charles Majkrzak (Neutron Condensed Matter Science Group, National Inst. of Standards and Technology (NIST)) at a symposium organized in his honor: The Development of Neutron Reflectometry and its Applications to Magnetism, Soft Matter, and Biology. The award recognized his seminal contributions to the development of neutron reflectivity and his pioneering work in applying his methods to many challenging problems. In particular, he designed, optimized, and made creative use of supermirror polarizers, integrating them into neutron instruments that attain very low backgrounds and consequently the highest signal-to-noise ratio achieved anywhere.



Uroporphyrinogen III Synthase

New Structures: Heidi Schubert (U. of Utah) solved 6 new crystal forms of *T. thermophilus* Uroporphyrinogen III Synthase generating 10 independent structures; the group had previously solved the human structure; and the RIKEN Structural Genomics/Proteomics Initiative (RSGI) solved two additional structures. The 7 most different structures were superimposed in the image on the previous page. Heidi described the flexibility of uroporphyrinogen III synthase alone and in complex with product and how flexibility relates to its cyclization of a linear tetrapyrrole, a required step for making heme. The tetrapyrrole cofactors support life systems through their essential catalytic functions: Heme (oxidative metabolism and oxygen transport); Chlorophyll (photosynthesis); Siroheme (sulfite and nitrite

assimilation); Cobalamin (vitamin B12 - methionine synthesis and methylmalonyl CoA synthesis) and coenzyme F430 (methane production). Their biosynthesis is complicated and requires anywhere from seven to 30 enzymatic reactions involving a variety of catalytic activities including decarboxylation, methylation, metal ion chelation and porphyrin ring oxidation. All five cofactors share their initial four synthetic steps, but at extended points in the pathways cofactor-specific branch points funnel intermediates towards their end product. *David Garboczi and Steve Ginell:*



The crystal structure of *Rhodobacter Sphaeroides* bc1 embedded in a modeled lipid bilayer. The surrounding membrane was computer generated; the membrane protein was placed into it, and overlapping lipids were removed. *Lothar Esser*

Membrane Proteins: Lothar Esser (NIH) described the 2.4 Å structure of a four-subunit bacterial bc1 complex (although no density is observed for subunit four). The asymmetric unit is very large, containing three dimers each of cytochrome b, cytochrome c1, and the iron sulphur protein. Density was observed for inhibitors, lipids, and detergent molecules. Although bacterial respiratory enzymes have proven more difficult to crystallize than their more complicated mitochondrial cousins, they offer unique views of the simplest way to establish the proton gradient necessary for ATP synthesis. *Susan Buchanan*

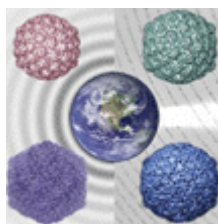
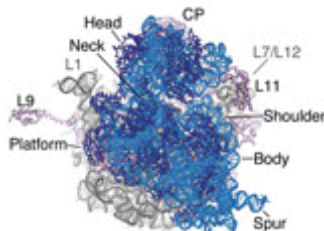


Figure by Lu Gan, reprinted from: Wikoff, W.R., Conway, J.F., Tang, J., Lee, K.K., Gan, L., Cheng, N., Duda, R.L., Hendrix, R.W., Steven, A.C., and Johnson, J.E. 2006. *J. Struct. Biol.* 153:300-6, © 2006, with permission from Elsevier.

Bio-Molecular Assemblies: below, from Jack Johnson (Scripps): A montage of four morphological forms of the bacteriophage HK97 capsid superimposed on the single crystal data (right) used to determine their structures and the solution scattering data (left) used to follow the transitions between forms. The earth is shown in the center to emphasize that bacteriophage constitute a significant fraction of the terrestrial biomass. *Hiro Tsruta and Volker Urban*



The structure of intact *E. coli* 70S ribosome at 3.5 Å resolution. View from the solvent side of the small subunit. 16S rRNA and proteins in the small subunit are light blue and dark blue, respectively. 23S rRNA and in the large subunit are gray and magenta, respectively. Reprinted from B.S. Schuwirth, M.A. Borovinskaya, C.W. Hau, W. Zhang, A. Vila-Sanjurjo, J.M. Holton, J.H.D. Cate, *Science*, (2005) 310, 827-834, with permission from *Science* © 2005.

Complementary Methods to Macromolecular Crystallography: Alex McPherson (UC-Irvine) gave an introduction to atomic force microscopy and its use to investigate everything from crystal growth to

the release of RNA from virus particles. The method provides nm resolution in the vertical direction of the scan and 2-3 nm resolution in the plane of the scan. AFM provides a detailed surface view of the objects investigated and it can be performed in solution. Quan Ho (Cornell) discussed small angle X-ray scattering (SAS) to determine molecular envelopes of macromolecules and the application of these envelopes for determining crystallographic phases. To do this the known envelope must be properly positioned and oriented in the crystal lattice. Bill Royer (U. Massachusetts) described time-resolved crystallography of hemoglobin, providing nano second time resolution and atomic spatial resolution of transitions that occur in the molecule as it loses its ligand and moves from the R to T state. The method requires a system that will repeatedly undergo the transformation in the crystal lattice and one that can be triggered by a laser. Andrew Stewart (Stony Brook U.), provided a progress report on the development of the X-ray microscope; Clare Peters-Libeu (Gladstone Inst., UCSF) presented a model for the human apolipoprotein E.DPPC obtained from crystallographic analysis of Bragg reflections and diffuse scattering as well as from SAS data; and Joshua Sakon (U. of Arkansas) described multiple methods, NMR, light scattering, size exclusion chromatography and thermal scanning calorimetry, to characterize the transition of the collagen binding domain of collagenase from the alpha to beta form. Jack Johnson (Scripps) finished the session by describing a 17Å resolution asymmetric cryoEM reconstruction of the bacteriophage P22. High resolution X-ray models of the tail spike proteins were readily fitted into the cryoEM density confirming the validity of the reconstruction. *Jack Johnson and Alex McPherson*

Connie Chidester



Charles Carter and Gerard Bricogne at the Opening Reception.