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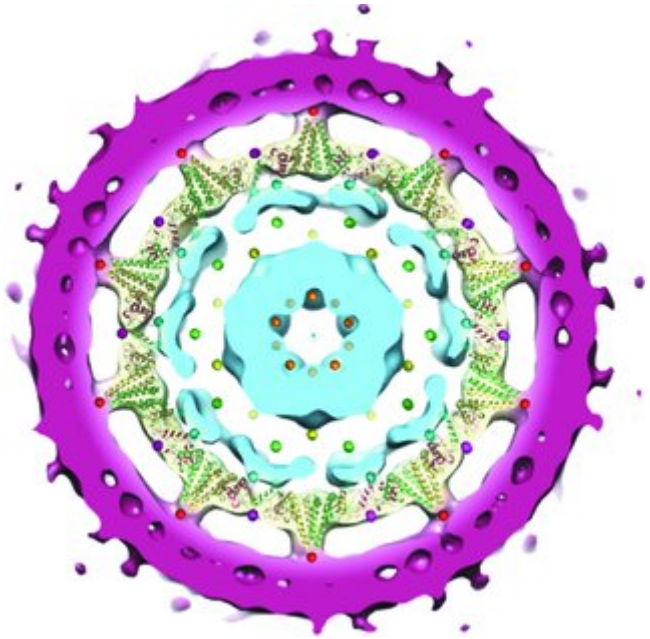
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IUCR JOURNALS NEWS

Molecular crystallography of icosahedral viruses

Acta Cryst. (2013). A69, 140-150 (http://doi.org/ksd); *Acta Cryst.* (2013). A69, 151-163 (http://doi.org/ksf)



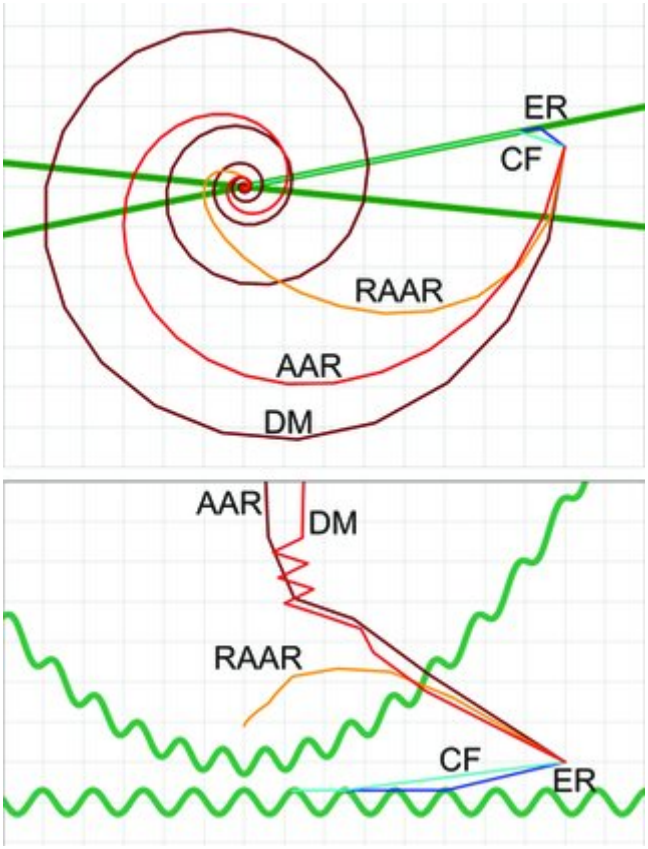
Model prediction correlates well with the three-dimensional structure of hepatitis B virus.
The exterior surfaces of icosahedral viruses are classified according to the T-numbers of Caspar and Klug, akin to crystal growth forms in crystallography. In analogy to the characterization of internal atomic structures of crystal growth forms *via* space groups, the interior organization of viruses is investigated here using icosahedral affine extensions by appropriate (indexed) translations. The analysis reveals a previously unrecognized structural interdependence of the shapes and sizes of different viral components, providing novel insights into structural constraints on virus architecture.

T. Keef, J. P. Wardman, N. A. Ranson, P. G. Stockley and R. Twarock; A. Janner

IUCR JOURNALS NEWS

The charge-flipping algorithm in crystallography

Acta Cryst. (2013). B69, 1-16 (http://doi.org/ksg)



Iteration paths of several dual-space algorithms for a convex consistent problem (upper panel) and non-convex inconsistent problem (lower panel). ER = error reduction, CF = charge flipping, DM = difference map, AAR = averaged alternating reflections, RAAR = relaxed averaged alternating reflections.

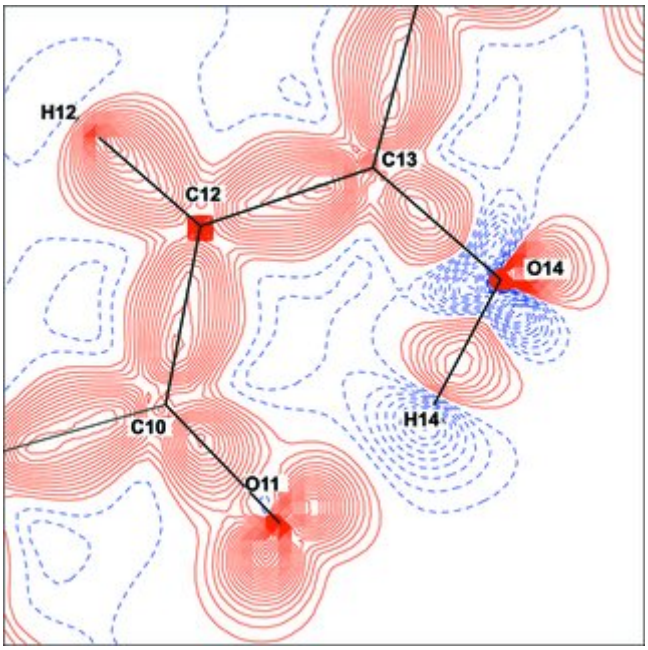
Dual-space iterative algorithms are conceptually simple, yet very efficient phasing algorithms applicable for solution of the crystallographic phase problem. Among the broad family of these algorithms the charge flipping algorithm (CFA) is the most widely used algorithm in crystallography. The article reviews the history of the dual-space algorithms in crystallography, the relationship of CFA to other dual-space algorithms, the variants of CFA, and the applications of CFA to routine structure solution, solution of aperiodic structures, powder diffraction data, macromolecular crystallography and single-particle imaging.

L. Palatinus

IUCR JOURNALS NEWS

Solid-state tautomeric structure and invariom refinement of a novel and potent HIV integrase inhibitor

Acta Cryst. (2013). C69, 285-288 (http://doi.org/ksh)



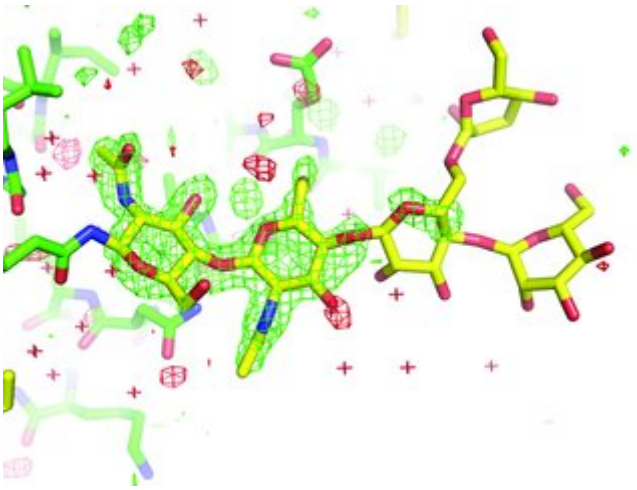
HIV-1 integrase catalyzes the integration of viral DNA into human chromosomal DNA, which is the 'point of no return' in an HIV infection. The conformation and tautomeric structure of a potent and novel integrase inhibitor with potential for HIV/AIDS therapeutics has been resolved. The electron-density distribution derived from invariom model scattering factors was a faithful mapping of the electron density in the crystal. The electrostatic potential of this molecule derived from the electron density could provide information on this molecule's ability to inhibit the activity of the integrase.

J. Bacsa, M. Okello, P. Singh and V. Nair

IUCR JOURNALS NEWS

Techniques, tools and best practices for ligand electron-density analysis and results from their application to deposited crystal structures

Acta Cryst. (2013). D69, 150-167 (http://doi.org/ksj)



Missing density: extended glycosylations. The specific conformation of the last three α-D-mannose moieties (A5-A7) of the extended branched glycosylation in PDB entry 3ib0 [Mir *et al.* (2009). *Biophys. J.* **97**, 3178-3186] is unsupported by electron density in the structure of bovine lactotransferrin, while the first two sugar moieties (A3-A4) are clearly present. The 1.4 Å resolution $mF_o - DF_c$ map contoured at +3σ (green) was calculated after refining a model omitting the sugar moieties of the glycosylation site.

Determining protein structures in complex with a small-molecule ligand is essential to the understanding of biologically important molecular interactions and in drug design. Electron density is the primary evidence which supports a particular ligand-binding mode in a corresponding complex structure. Inspection of deposited structure models reveals low real-space correlation coefficients for a large number of small-molecule ligands. Several classes of detected problems are analyzed, and suggestions for improvement in training of crystallographers and model validation are provided.

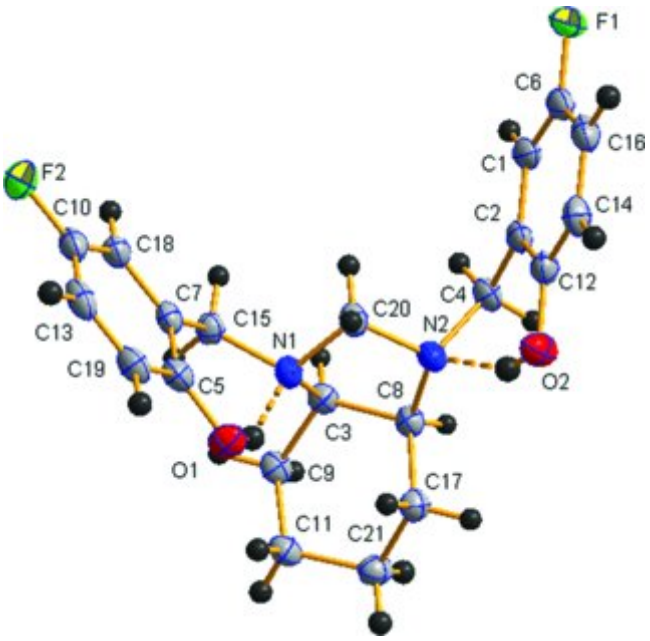
E. Pozharski, C. X. Weichenberger and B. Rupp

IUCR JOURNALS NEWS

meso-4,4′-Difluoro-2,2′-{[(3aR,7aS)-2,3,3a,4,5,6,7,7a-octahydro-1H-1,3-benzimidazole-1,3-diyl]-bis(methylene)}diphenol

meso-4,4′-Difluoro-2,2′-{[(3a*R*,7a*S*)-2,3,3a,4,5,6,7,7a-octahydro-1*H*-1,3-benzimidazole-1,3-diyl]-bis(methylene)} diphenol

Acta Cryst. (2013). E69, o217 (http://doi.org/ksk)



A perspective view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Hydrogen bonds are drawn as dashed lines.

In 1,1-diamines the conformations are strongly disfavored if the unshared electron pairs on nonadjacent N atoms are parallel or syn-axial. The consequences are seen in the preferred conformation of certain heterocyclic rings. Eliel proposed to call this phenomenon the 'rabbit-ear effect'. The crystal structure of the title compound established the existence of a 'rabbit-ear effect' in the N-C-N aminal motif in which the lone pairs of the N atoms are located in syn disposition. The title compound is a good model to study intracyclic stereoelectronic effects.

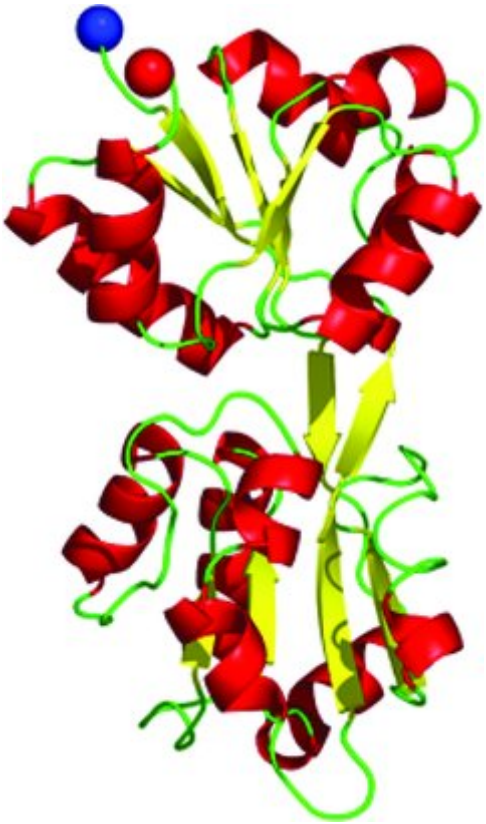
A. Rivera, D. Quiroga, J. Ríos-Motta, M. Kuceraková and M. Dusek

IUCR JOURNALS NEWS

The AEROPATH project targeting Pseudomonas aeruginosa: crystallographic studies for assessment of potential targets in early-stage drug discovery

The AEROPATH project targeting *Pseudomonas aeruginosa*: crystallographic studies for assessment of potential targets in early-stage drug discovery

Acta Cryst. (2013). F69, 25-34 (http://doi.org/ksm)



Crystal structure of HemD from the pathogen *Pseudomonas aeruginosa*. The enzyme is located at a metabolic branching point leading to the biosynthesis of haem, sirohaem or vitamin B_{12}.

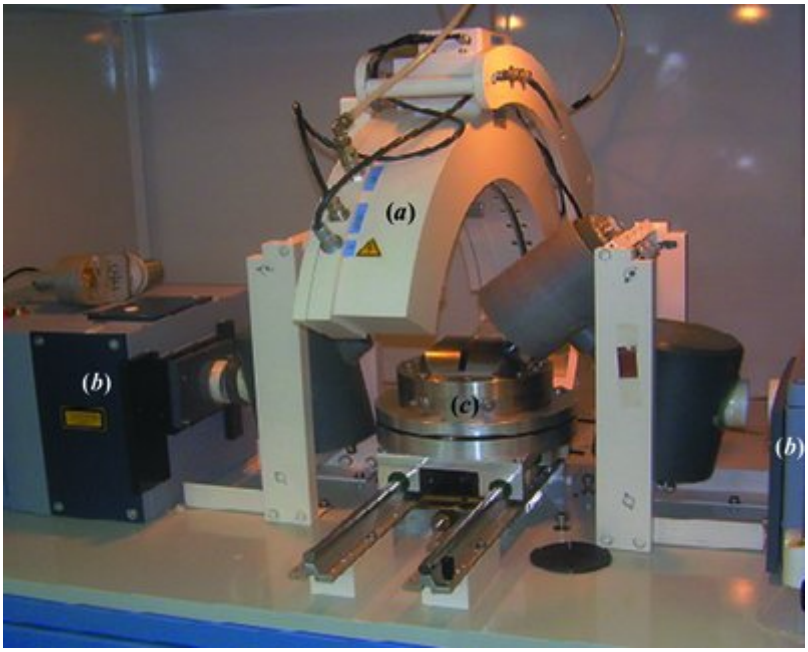
Bacteria, particularly Gram-negative species, present a serious challenge to human health. At worst, increasingly antibiotic-resistant pathogens threaten to undo over half a century of medical progress. Traditionally, antibiotics were discovered empirically through large screening efforts of natural products. The power of modern structural biology allows antibiotic discovery to start with atomic resolution information of potential drug targets. Here, we report a suite of protein crystal structures from the pathogen *Pseudomonas aeruginosa* that provide rational starting points for future antibiotic discovery.

L. Moynie, R. Schnell, S. A. McMahon, T. Sandalova, W. A. Boulkerou, J. W. Schmidberger, M. Alphey, C. Cukier, F. Duthie, J. Kopec, H. Liu, A. Jacewicz, W. N. Hunter, J. H. Naismith and G. Schneider

IUCR JOURNALS NEWS

An X-ray diffractometer coupled with diffuse reflectance infrared Fourier transform spectroscopy and gas chromatography for in situ and in operando characterization: an innovative analytical laboratory instrument

J. Appl. Cryst. (2013). 46, 262-266 (http://doi.org/ksn)



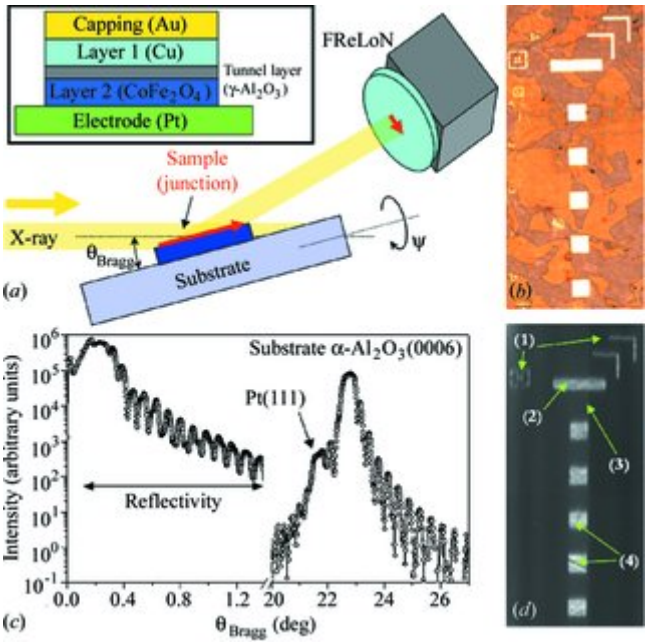
For the first time, an innovative reaction cell allowing simultaneous XRD and DRIFT spectroscopy characterizations has been developed for *in situ* and *in operando* applications at a laboratory scale. Thanks to the high temperatures (873 K) and high pressures (18 bar) supported, this tool, associated with an online gas chromatograph, is well adapted to heterogeneous catalysis as chemical reactions take place at the surface of the material and can be influenced by its structure.

L. Braconnier, I. Clémençon, C. Legens, V. Moizan, F. Diehl, H. Pillière, P. Echegut, D. De Sousa Meneses and Y. Schuurman

IUCR JOURNALS NEWS

X-ray diffraction imaging of metal-oxide epitaxial tunnel junctions made by optical lithography: use of focused and unfocused X-ray beams

J. Synchrotron Rad. (2013). 20, 355-365 (http://doi.org/ksp)



Schematics of the X-ray diffraction imaging experiment and the model sample used (epitaxial magnetic tunnel junction).

Metal-oxide magnetic tunnel junctions, consisting of an insulating layer sandwiched between two electrodes made of hard and soft ferromagnetic layered materials, are highly sensitive sensors for spintronic applications. Typical sizes in the micrometre range favored investigations using X-ray imaging techniques. The layers, differing either by their lattice parameter or by crystalline structure, were easily distinguishable from each other by X-ray diffraction contrast, while raster imaging and local probe diffraction allowed defects and distortions at both the macro- and the microscale to be detected and localized.

C. Mocuta, A. Barbier, S. Stanescu, S. Matzen, J.-B. Moussy and E. Ziegler

FEATURE ARTICLE

Member Profile and Favorite Crystal



Gautam Desiraju

I was trained as a physical organic chemist before I studied crystallography. My research has always been influenced by these two subjects during my independent career that has so far lasted 33 years. I have tried to look at what determines the crystal structure of a small organic molecule and whether or not one can predict such crystal structures using experimental, computational, or database-related methods. These goals constitute a part of the subject of crystal engineering. This subject today also has come to include an understanding of the process of crystallization. Crystal nucleation is not studied as well as crystal growth. How and why do crystals nucleate? I do believe that such challenging themes will play a natural part in the future of crystallography.

After the landmark studies of Max von Laue and the Braggs, father and son, 100 years ago, crystallography changed from being a subject pertaining to the study of crystals to a study of the determination of the internal structures of crystals from their diffraction patterns. I believe that the phase of research that dealt with structure determination of crystals from their diffraction patterns is now coming to a close. Crystallography will undoubtedly see newer avenues for its progress. One of these will be the study of the crystallization event itself. How does long-range order enter the crystal nucleus? Does a crystal nucleate from an amorphous precursor? Clearly these are questions that cannot be answered with diffraction alone. We also need spectroscopy and computation in big ways to solve these problems. One might also want to redefine what a crystal is to include all species with some degree of order.

My personal goals for the International Year of Crystallography (IYCr) are that it should allow crystallographers to reinforce a sense of group identity and to convey their enthusiasm for this remarkable subject to the larger scientific community. Science brings people together and I believe that the IYCr should be an occasion for us to try and foster relationships between scientists in different countries or in different regions of the world. Because of the universality of science it is natural that scientists from different parts of the world come together, setting aside cultural, social, religious and economic differences that may be otherwise prevalent, and which tend to separate people. The IYCr I believe should also be an occasion when scientists are able to explain to the general public, and also to students and younger people, about the excitement and importance of crystallography as a scientific endeavor.



Srirangam Temple



The Orlov diamond

I and others have been asked by the Editor of the IUCr Newsletter to mention what I consider to be the most important crystal ever found or grown and why it is important. Any such choice will quite necessarily be subjective and therefore it is difficult to provide a justification beyond a certain level. Anyway, my choice of a favorite crystal is diamond, for both scientific and personal reasons. Till a few hundred years ago all the diamonds in the world were mined in my country. A great number of very famous diamonds like the Koh-i-Noor and the Hope, which intertwine history, geopolitics and intrigue, originate from the famous mines of Golconda, which is not very far from the campus of the University of Hyderabad, where I lived and worked for 30 years. Diamond is one of the earliest crystals whose crystal structure was determined from its diffraction pattern. It was a crystal that greatly impressed C. V. Raman, who referred to it as the prince of solids. I am fascinated by what might, in the end, be called its 'fearful symmetry'. Many questions can be posed about this remarkable crystal. Why is hexagonal diamond, or Lonsdaleite, so uncommon compared to its cubic counterpart? Why is its thermal conductivity so high? Why is it so hard? Why and how do trace gases get occluded in this crystal, giving rise to the remarkable range of color that is observed? As an organic chemist, I could call diamond the 'ultimate cyclohexane' and in this regard its topology is an attractive target for supramolecular synthesis. The diamond network is actively pursued by crystal engineers who work both with pure organics and with metal-organic framework (MOF) compounds.

Ancient Indian writings refer to diamonds as crystals and the ancient Hindu word for diamond is related to the words for thunder and lightning. As early as the third century BC, the octahedral shape of the diamond crystal was noted in India and archeologists have found evidence of diamond-tipped drills from around that time. I have enclosed a picture of the famous Orlov diamond, presently in the Kremlin in Moscow but located till the early 18th century in the Ranganathaswamy temple in Srirangam, Tamil Nadu, India, where it was once one of the eyes of the presiding deity. The Orlov diamond was also mined in Golconda and is preserved in its, currently rare, original cutting that was a specialty in medieval India.

G. R. Desiraju

MEETING REPORT

ACA 2012

Boston, MA, USA, July 2012
www. amercrystalassn.org
taken from ACA RefleXions, Fall 2012

Continued from Volume 20, Number 4

Exciting Structures



Speakers in Exciting Structures. Front row: Hua Li, Jason Stagno, Sozanne Solmaz, Sung-il Yoon, Dinesh Yernool. Back row: Eric Armstrong, Dirk Zajonc, Douglas Davies, Charles Dann, Graeme Conn.

J. Stagno (NCI) described the first RNA supercoil structure ever observed. As in most nucleic acid-containing crystals, the double-stranded RNA duplexes form pseudo-continuous helices. However, Stagno's helices adopt a coiled-coil plectonemic RNA supercoil, mediated by the RNA binding protein NusB. This remarkable structure provides novel insights into high-density nucleic acid structures, suggesting how protein-mediated RNA supercoiling may facilitate the packaging of viral RNA genomes.

D. Yernool (Purdue) presented studies of a DNA-protein complex from a bacterial two-component signal transduction system, shedding light on the mechanism by which the phosphorylation signal is communicated, the role of interdomain surfaces in regulation of gene expression, and the basis of the increased affinity of activated RRs for DNA.

D. Davies (Emerald Bio) described the first structure of an *in vitro* evolved 'SOMAmer' (slow off-rate modified aptamer) in complex with its protein target. SOMAmers expand the chemical diversity of nucleic acids through incorporation of modified groups such as amino acid-like side chains. This SOMAmer binds its target protein (a growth factor) through shape complementarity and hydrophobic interactions, mimicking the interaction of the target protein with its receptor. The structure may help identify high-affinity ligands for proteins that are recalcitrant to selection using standard nucleic acids.

S. Solmaz (Rockefeller U.) described her ambitious effort to model the transport channel of the nuclear pore complex. Her model of the entire transport channel, a 12.3 MDa complex, adhered to its overall shape and symmetry determined by electron microscopy, accounts for the remarkable range of pore dynamics necessary for the accommodation of a wide variety of cargo sizes. Her movie showing the contraction of the channel's ring diameter from ~40 nm to ~20 nm, with a concomitant 150% increase in height from 4 nm to 6 nm, was a session highlight.

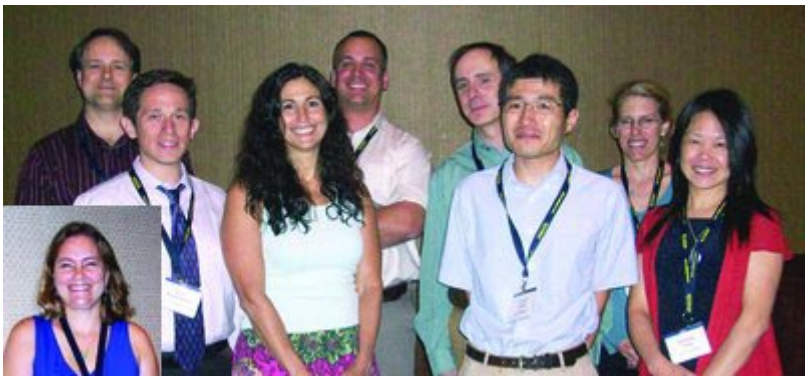
H. Li (UT Southwestern Medical Center) presented recent studies of the sodium/calcium exchanger (NCX) and a welcome foray into the field of electrophysiology. Li finds one Ca and three probable Na binding sites clustered at the center of the outward-facing NCX from *Methanococcus jannaschii*, and two channels where extracellular ions could gain access to these sites. S. Yoon (Kangwon National U.) presented the first and only structure of a toll-like recepter (TLR) bound to a ligand, the D1-D2-D3 domain of *Salmonella* flagellin. Rearrangement of a protruding loop within TLR facilitated flagellin accommodation within the binding pocket and resulted in subsequent dimerization of the complex *via* the receptor's C-terminal tails, allowing downstream activation to ensue.

D. Zajonc (La Jolla Inst. for Allergy and Immunology) focused on glycolipid antigen recognition by type 1 *versus* type 2 natural killer T (NKT) cells. Many of the key residues responsible for T-cell recepter (TCR) binding were shown to be conserved in other known sulfatide-reactive TCR's, suggesting a common structural modality that enables recognition of this class of self-antigens.

C. Dann III (Indiana U.) talked about the potential of novel antifolates to target the human folate receptor (hFR) and extend this class of therapeutics into a new generation of cancer treatments. Dann described a membrane-anchored protein in its apo form and with folates and antifolates bound and at acidic and neutral pH. By designing drugs whose sole entry into cells occurs *via* the hFR endocytic pathway, they hope to circumvent the dose-limiting toxicity of traditional antifolates.

Eric Armstrong and Graeme Conn

Enzyme Mechanisms

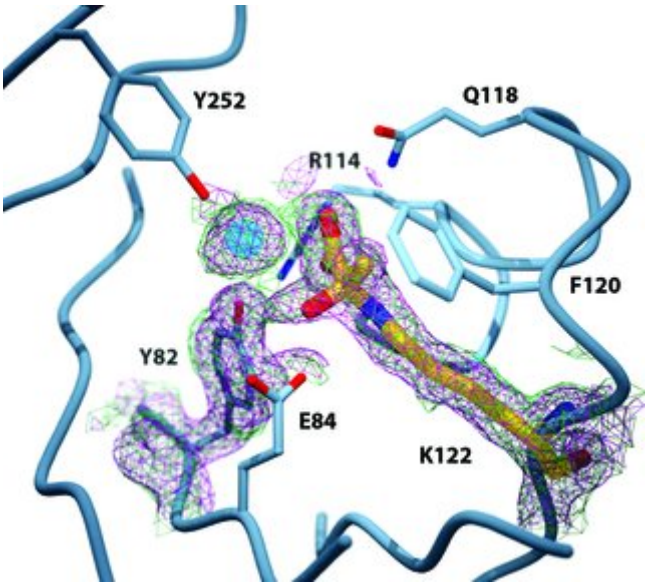


Speakers in Enzyme Mechanisms. Zachary Wood, Eric Montemayor, Karen Allen, Nicholas Silvaggi, Adrian Goldman, Hideki Aihara, Rebecca Page and Xiaojing Yang. Inset: Catherine Drennan.

C. Drennan (MIT) described the long-awaited structure of the protein components required for the methyl transfer from folic acid (vitamin B9) to vitamin B12, a reaction necessary for acetogenesis. Her structure revealed the conformational changes required for the methyl transfer between these B vitamins. H. Aihara (U. of Minnesota) discussed a eukaryotic DNA repair enzyme TDP2 that plays a critical role in resistance to DNA damage, and is a potential drug target for chemotherapy. The structure of TDP2 and the mechanism of its substrate recognition have been elusive. The Aihara laboratory determined the structures of TDP2 in the presence and absence of DNA substrate. TDP2 has a narrow groove that selectively accommodates the 5′-terminus of a single-stranded DNA, a novel mode of DNA binding. R. Page (Brown U.) discussed how ser/thr phosphatases (PSP) achieve specificity in the cell. Although more than 420 genes in the human genome encode for serine/threonine kinases, less than 40 genes encode for PSPs. Most PSPs are tightly regulated by their interaction with targeting and inhibitor proteins. Page described her PP1:targeting and CN:inhibitory protein complexes, showing PSP interacting proteins direct PSP activity via inhibition of substrate sites rather than the active site. E. Montemayor (UT Health Science Center-San Antonio) discussed the intron debranching enzyme (Dbr1) in complex with several RNA compounds that mimic the branchpoint structure in lariat RNA. A combination of cell-based functional assays, *in vitro* activity assays, inductively coupled plasma mass spectrometry and X-ray anomalous diffraction methods were used to support a new proposal for the mechanism of Dbr1, in

which a dinuclear metal-binding center alternates between single and double metal ion configurations. The findings clarify the role of Dbr1 in retrotransposon and retrovirus replication, and suggest evolutionary relationships between retrotransposons, retroviruses and pre-mRNA splicing.

X. Yang (U. of Chicago) uses temperature to trap reaction intermediates in phytochromes that convert a light signal into a biological signal *via* reversible photoconversion between red-absorbing (Pr) and far-red-absorbing (Pfr) states. Xiaojing used temperature-scan cryocrystallography on photoactive crystals of *P. aeruginosa* BphP (PaBphP). By applying a trap-pump-trap-probe strategy, they followed the progression of photoreaction in the crystalline state. The higher the pump temperature, the greater the structural relaxation and the further the reaction proceeds. Light-induced difference electron densities at ten temperatures were analyzed, from which three cryo-trapped intermediate structures in the Pfr-to-Pr photoreaction were delineated.



Investigations of two enzymes from family V of the ADCSF.
Z. Wood (U. of Georgia) showed that a large conformational change in a protein can be caused by a small allosteric effector. When the allosteric inhibitor UDP-α-D-xylose binds to the active site of human UDP-α-D-glucose-6-dehydrogenase (hUGDH), the active hexamer is converted into an inactive U-shaped complex, supporting an evolutionary model in which catalytic efficiency is sacrificed to select for unstable hexameric complexes. Combining biochemical and sedimentation velocity studies, Wood finds apo-hUGDH to be a tipping point between the active and inactive states. Apparently, nature selected for a conformation that is suboptimal for catalysis in order that the small chemical difference between the allosteric inhibitor and the substrate can be a conformational switch.

A. Goldman (U. of Helsinki) presented the first sodium-pumping inorganic pyrophosphatase structure, an integral membrane protein from *T. maritima* (TmPPase). TmPPase has 16 transmembrane helices, all of which extend up to 20 Å above the membrane surface on the cytoplasmic side. An inner ring of six helices forms the hydrolytic centre, coupling the channel to a gate (just below the membrane) and the exit channel.

N. Silvaggi (U. of Wisconsin-Milwaukee) discussed bioinformatic analysis of enzymes in the acetoacetate decarboxylase superfamily (ADCSF), and identification of families having active-site architectures distinct from the prototypical decarboxylases. Members of this family have a new type fold and aldolase activity.

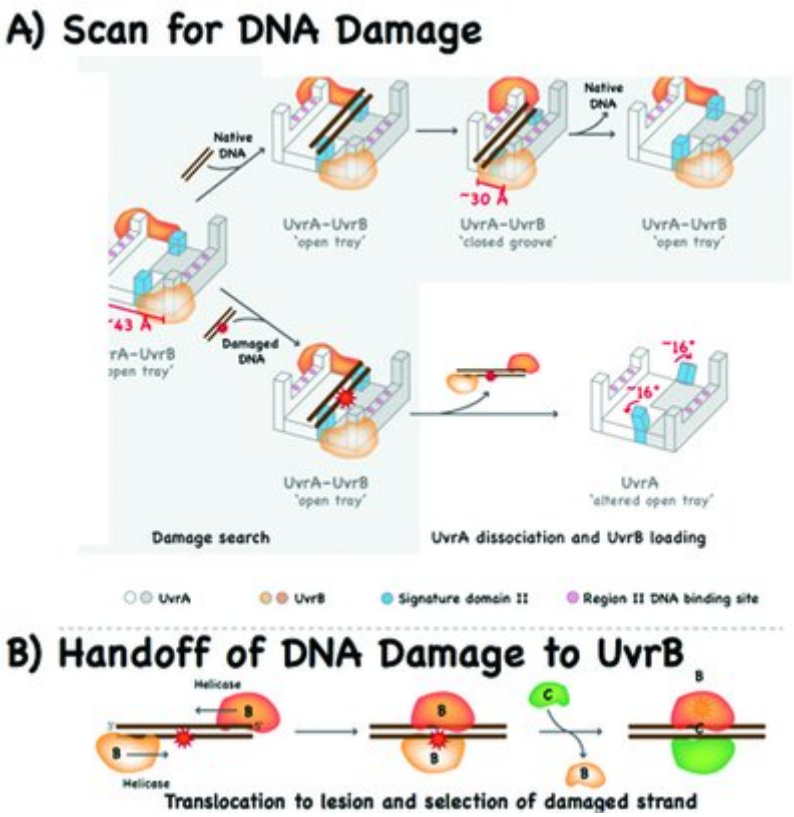
Karen N. Allen

Structural Enzymology - Biology



Speakers in Structural Enzymology. Front row: Cynthia Stauffacher, Flora Meilleur, Celia Goulding, and Philip Anfinrud. Back: Savvas Savvides, David Jeruzalmi, Sean Froese, Brandt Eichman, William Royer, Zachary Wood. Inset: Liang Tang.

P. Anfinrud (NIH) revealed the power of ultrafast time-resolved SAXS/WAXS technology to observe real-time protein conformational changes in solution. He described changes in protein size and shape as photoactive yellow protein (PYP) underwent a photoactivated signaling-state transition. The transition involved a structural change that cannot be accommodated in protein crystals but can be detected by time-resolved Laue crystallography studies in which the PYP chromophore changes from a red-shifted to a blue-shifted spectroscopic intermediate. A water molecule penetrates into the interior of the protein where it forms hydrogen bonds that temporarily block the ground state recovery of PYP. The ability to track large-amplitude structural changes in solution *via* time-resolved SAXS/WAXS is proving to be a powerful complement to time-resolved Laue diffraction studies.



Ribbon representation of the BARF1:hCSF-1 complex. Hexameric BARF1 binds three hCSF-1 dimers. The oligo-mannose type glycan structures are shown in stick and surface representation. Adapted from Elegheert *et al.* (2012), *Nature Structural and Molecular Biology* (doi 10.1038/nsmb.2367).

S. Savvides (Ghent U.) used biophysical and crystallographic approaches to reveal the mechanism by which the viral decoy receptor BARF-1 from the Epstein-Barr virus hijacks our immune system. Savvides

found that viral BARF-1 binds CSF-1 at an epitope far from that of the cognate human receptor and locks CSF-1 into a conformation that is unable to bind and signal *via* the cognate receptor.

C. Goulding (U. California-Irvine) discussed contact dependent growth inhibition (CDI) systems of gram-negative bacteria. CDI occurs when the C-terminal tail of CdiA, CdiA-CT, a toxic protein, is translocated into a target cell to inhibit growth. Related bacteria express immunity proteins (CdiI) that neutralize the CdiA-CT proteins. Goulding's structures of two CdiA-CT/CdiI complexes show that the CdiA-CT toxins are structurally similar, despite very low sequence conservation. However, one is a tRNase and the other a Zn^{2+}-dependent DNase. In contrast, the CdiI's are nonhomologous structures, showing that the immunity factors have distinct origins in evolution.

D. Jeruzalmi (Harvard U.) described the nucleotide excision repair pathway (NER) in bacteria, the DNA damage sensor from the NER pathway, and how the sensor may identify the presence of UV damage on DNA. Three crystal structures of various components in the pathway, combined with known biochemistry, provide details of early steps of NER. DNA (native and damaged) is sampled by the open form of UvrA, and sampling involves closing around the DNA to sense its shape. Native DNA passes this airport-style 'pat-down' and is released. Damaged DNA fails the test, and is shunted to the damage-specific stages of the pathway.

B. Royer (U. Mass Medical School) used time-resolved crystallography and meta-analysis of 70 structures to follow cooperative conformational change in the dimeric hemoglobin HbI and reveal the role of water molecules in facilitating the transition between R and T states, in which the helices of the different subunits undergo a scissoring motion to facilitate the cooperative transition between states. B. Eichman (Vanderbilt U.) revealed how the DNA repair enzyme AlkD adopts an unusual conformation that exposes alkylated purines and facilitates base excision, despite the absence of a direct chemical contact between the enzyme and the labile glycosidic bond, a nice explanation of how the DNA itself can facilitate catalysis in a DNA repair enzyme.

F. Meilleur (North Carolina State U.) described IMAGINE, a high-intensity neutron diffraction beam line that will begin operations next spring at ORNL. Flora discussed neutron diffraction studies of xylose isomerase, an enzyme of interest to the biofuel community. L. Tang (U. Kansas) explained how the bacteriophage Sf6 accomplishes the difficult task of packaging DNA into the viral capsid. The terminase is a large protein complex that pumps DNA through the portal protein channel into the capsid, powered by ATP hydrolysis. The terminase small subunit called gp1 assembles into a ring-like octamer and binds the DNA in nucleosome-like fashion, to select viral DNA for packaging. S. Froese (U. Oxford) described details of glycogen biosynthesis, including how the glycogen core protein, glycogenin, nucleates the synthesis by forming a covalent Tyr-glucose bond, and how conformational changes in the catalytic core of the protein and the growing maltosaccharide chain are important to the reaction. He also proposed a mechanism for the glycogen storage disorder XV in which Thr83Met mutation locks the enzyme in a conformational state that is not catalytically competent to initiate glycogen biosynthesis.

Zachary Wood and Cynthia Stauffacher

Functional Nanomaterials



Speakers in Functional Nanomaterials. Alamgir Karim, Detlef Smilgies, Volker Urban, Kevin Yager and Tad Koga.
Speakers in this session described the study of electronics, piezoelectrics, photo-voltaics and other nano-materials using various techniques including grazing-incidence methods (GISAXS, GIWAXS, and GI-XPCS) that measure thin films.

A. Karim (U. of Akron) described the use of localized but moving hot bands (zone annealing) to control block-copolymer (BCP) nanoscale morphology. Zone annealing can enhance ordering kinetics and orient microphases. Karim demonstrated that extremely sharp thermal gradients enable better control of order and orientation. Optimized annealing can maintain a vertical orientation for the BCP cylinder phase in films up to 1000 nm thick. The process was further refined by adding a polymer (PDMS) capping layer to the thin film being zone annealed. This flexible layer induces in-plane shearing at the film-PDMS interface and is dubbed 'soft-shear' that induces alignment of the BCP layer over the entire macroscopic dimensions of the sample. This remarkable ordering was confirmed using AFM images and GISAXS analysis.

D. Smilgies (CHESS) presented GISAXS and GIWAXS studies of the ordering of thin films, including *in situ* measurements conducted during film formation. The assembly of oleic acid-coated PbS spheres from solution into films was pathway-dependent. The solvent evaporation rate affected assembly and could be tuned continuously between FCC and BCC superlattices. Shape anisotropy of spherical nanoparticles drove rearrangement of the superlattice; the particles become oriented within the lattice, as confirmed by WAXS measurements. Process history (solvent evaporation, temperature and annealing history, shear *etc.*) plays an important role in determining the final nanostructure order of thin-film nanomaterials with potential industrial applications.

Tad Koga and Kevin G. Yager

Macromolecular Science with Scattering Methods



Speakers in Macromolecular Science with Scattering Methods. Front: Tobin Sosnick, Angela Criswell, Rick Russell, Mark Del Campo; back: Kwaku Dayie, Xianyang Fang, Osman Bilsel, Michal Hammel, Xiaobing Zuo.
Solution X-ray scattering (SAXS) has become a major tool for structural biology, brought about by the development of high-flux X-ray sources, large area detectors, and data analysis methods and programs. T. Sosnick (U. Chicago) found that single-molecule fluorescence resonance energy transfer (smFRET) and SAXS produce divergent views of the unfolded states at low denaturant concentrations. SmFRET experiments suggest the chemically unfolded proteins invariably collapse from random coil to more compact dimensions as the denaturant concentration is reduced, while SAXS experiments suggest that such compaction may be rare. The possible cause of this discrepancy was discussed.

R. Russell (U. Texas-Austin) described the interactions between unstructured RNAs and DEAD-box ATP-dependent chaperones that can unwind short helices in structured RNAs and refold the kinetically

trapped intermediates.This flexible positively charged tail interacts non-specifically with nucleic acid, tethers the protein to the structured RNA and directs the chaperone protein toward helical unwinding.

X. Fang (NCI-Frederick) described an HIV Rev response RNA element (RRE RNA), that binds to Rev protein to export viral genes from the nucleus to the cytoplasm, which overwhelms the host's defenses. Two Rev protein binding sites, 60 Å from one another, foster oligomerization of Rev proteins for viral gene export. T. K. Dayie (U. Maryland,) described SAXS and NMR studies of SAM-riboswitch RNAs, in which the Shine-Delgano sequence is buried in a pseudo-knot conformation in the apo-form and exposed in the bound form to allow gene expression.

M. Hammel (LBNL) described the highly automated BioSAXS setup and services provided at the SIBLYS beamline FOXS, a program that calculates scattering profiles using the Debye formula. O. Bilsel (U. Mass) described a continuous turbulent flow-based time-resolved BioSAXS setup with BioCAT at Argonne that allows observation of early stages of biomolecular folding processes that would be inaccessible by stopped-flow techniques. M. Del Campo (Rigaku Americas) described a home laboratory SAXS instrument with focusing optics that provides usable data in 5 min to 2 hours with reasonable signal-to-noise.

Xiaobing Zuo and Angela Criswell

Complementary Techniques in Structural Biology



Speakers in Complementary Techniques in Structural Biology. Front: David Case, Allan Pang, Arwen Pearson, Allen Orville; back: Joseph Yarbrough, Dagmar Ringe, Lesa Beamer, Edward Snell, Nozomi Ando. Inset: Agnesa Shala.

D. Case (Rutgers U.) described extending molecular dynamics simulations from individual molecules to crystal lattices for small peptides and showed clear potential to improve solvent modeling in macromolecular structures. A. Orville (BNL) showed how combining single-crystal spectroscopy, diffraction and X-ray fluorescence was providing a picture of nitrogen fixation in root nodules. J. Yarbrough (U. Florida), an undergraduate recipient of an ACA Travel Award, used circular dichroism and differential scanning calorimetry to follow the unfolding of a viral capsid induced by pH variation. N. Ando (MIT) used SAXS, X-ray crystallography, electron microscopy and analytical ultracentrifugation to show that ribonucleotide reductase existed as a mixture of transient species with distributions modulated by allosteric effectors. Each technique supported evidence from the others and provided unique information, completing the overall picture of the structural mechanism.

Combining structural information with theoretical predictions of perturbed titration curves for individual amino acids, D. Ringe (Brandeis U.) showed how residues outside the active site can control reactivity. Lesa Beamer (U. of Missouri) combined NMR and crystallographic information into context and to better understand connections between structure, dynamics and catalysis in phosophohexomutase. Etter lecturer A. Pang (Queen Mary U.) discussed bacterial metabolosome structures formed from hexagonal-shaped tiles made up of different protein subunits. A. Shala (York U.) presented bioinformatic approaches

combined with affinity pull-down assays and mutagensis to study periplasmic proteins linked to antibiotic resistance in human pathogens.

Eddie Snell and Arwen Pearson

Important Science from Small Molecule Structures



Speakers in Important Science from Small Molecule Structures. Larry Falvello, Alberto Albinati, Lawrence Dahl, Mike Hall, Bruce Foxman, Alan Pinkerton, Lee Daniels, Silvia Chiara Capelli, Mark Bowden.
The focus of this session was cluster chemistry, hydrogen storage, topotaxy, displacement parameters, experimental and theoretical electron densities, and reaction mechanisms. L. Dahl (U. Wisconsin) addressed complex bonding questions in his family of Pd clusters, such as the stabilizing influence of an inert electron pair in Tl(I)/Pd(0) compounds. M. Bowden (Pacific North West National Laboratory) discussed boron adducts which have a greater mass density of hydrogen (~140 g/l) than does liquid H_2 (~70 g/l). M. Hall (Texas A&M) adressed quantum chemistry and structural aspects of reaction mechanisms in transition metal complexes. He described density functional theory (DFT) as a free lunch, because the quality of the results obtained from properly used DFT is disproportionate to the relative ease with which the calculations can be done. He pointed out that it is possible to get variable results using different functionals and cited a case of an intermediate predicted by DFT, though not experimentally observed. A Pinkerton (U. of Toledo) provided a bridge between theory and high-resolution diffraction analysis with a charge-density study of croconic acid, a high-density organic (ρ = 1.912 g/cm^3) which is ferroelectric at and above room temperature. The charge-density analysis explained the intermolecular interactions observed in croconic acid. S. Capelli (Inst. Laue-Langevin) described several applications of normal-mode analysis from mean-square atomic displacement amplitudes, including applications to urea and sucrose, for which the results agree with data from terahertz spectroscopy. Capelli emphasized the distinguishing characteristics of neutron diffraction; elemental contrast distinct from that of X-ray diffraction, scattering lengths independent of resolution, and hydrogen scattering, so much more powerful than scattering by electrons. B. Foxman (Brandeis U.) described thermally induced topotactic reactions and the method of establishing the geometrical relationship between different phases oriented under the same conditions without removing the crystal from the diffractometer.

Alberto Albinati, Lee Daniels, and Larry Falvello

Cool Structures



Speakers in Cool Structures. Front: Ying-Pin Chen and Elena Forcen-Vazquez, back: Allen Oliver, Lorraine Malaspina, Kevin Gagnon, Faye Bowles, Chun-Hsing Chen, James Hall, Xiaoping Wang.
J. Hall (U. Reading, UK) described DNA intercalation by Ru complexes in a variety of bonding modes. Both Delta and Lambda forms of the complex were found to interact with DNA decamer chains in each of three bonding modes. E. Forcen-Vazquez (U. of Zaragoza) discussed polymeric diversity in copper citrate complexes ranging from one-dimensional chains to three-dimensional extended networks, some of which are single-molecule magnets. Hydration can affect the polymer formation and produce different networks. J. Chen (Indiana U.) synthesized large cyclic structures, cyanostars, from cyano-stilbene, that have cavities suitable for capture of anions of specific sizes. Having five-fold symmetry, these cyanostar complexes pose crystallographic challenges, including disorder. Chen demonstrated how this disorder was resolved.

K. Gagnon (Texas A&M) described one-dimensional inorganic-organic hybrid materials (alkylbisphosphonic acids and zinc acetate), in which chains of tetrahedral zinc atoms cross-linked by octahedral metal atoms form nanometer-size one-dimensional tunnels filled with disordered solvent molecules. The channel size and shape are sensitive to small variations of zinc site occupancy. L. Malaspina (U. Fed Goias) discussed analysis of the disordered structure of a coumarin ester of ambiguous space group. Y.-P. Chen (Texas A&M) discussed controlling the topology of metal organic framework (MOF) structures by changing the molar ratios of the reaction precursors in solution and changing solvent combinations. Chen provided several examples of different MOF frameworks composed of the same building blocks. F. Bowles (UC Davis) discussed cleavage of metal-metal bonds by reaction of metal-metal bonded carbonyl complexes with C_{60} to produce a new metal-fullerene adduct.

Allen Oliver and Xiaoping Wang

Magnetic Materials



Speakers in Magnetic Materials. Ovidiu Garlea, Ashfia Huq, Susan Herringer, Simon Parsons, Timothy Munsie, John Greedan, Dimitry Khalyavin.
Sponsored by Materials, Neutron and Powder SIG, this session featured materials synthesis, molecular magnets studied under pressure and three different families of compounds which have exciting magnetic properties. J. Greedan (McMaster U.) discussed short- and long-range magnetic order observed in vacancy ordered/disordered perovskite structures. D. Khalyavin (ISIS) described exchange topology in the hexagonal lattice system $R BaCo_4O_7$, where geometrical frustration gives rise to varied degrees of spin correlation. O. Garlea (ORNL) described the effect of oxygen doping on the structural and magnetic properties of delafossite compounds. The session included studies of molecular-based magnets under pressure, effects of random exchange in ferromagnetic copper chloride chains, and studies of single-crystal holmium titanate.

Ashfia Huq

Prions, Amyloids and 'Friends'



Speakers in Prions, Amyloids and 'Friends'. Front: Christopher Stanley, Gerald Stubbs, William Wan, Hiromi Arai; back: Joseph Orgel, Robyn Stanfield, Sankar Naravan Krishna, Wenji Zheng.

Prions and amyloids are the root cause of or directly associated with systemic and neurological diseases such as Alzheimer's, Parkinson's and Huntington's. J. Orgel (Illinois Inst. of Tech.) provided a brief overview of pathological fibril-forming peptides. C. Stanley (ORNL) presented a time-resolved neutron scattering study of the aggregation kinetics of huntingtin amyloid precursors, revealing a clear distinction between the wild-type and pathological forms of the protein. Using fiber diffraction, Etter Lecturer W. Wan (Vanderbilt U.) detected structural polymorphism in the fungal prionizable element HET-s. When fibrils from this peptide are formed at pH 7.5 they do not display infectious qualities. Fibrils formed at pH 2 do. Significant degradation occurs at low pH, which may well account for the different (and infectious) structure of the HET-s fibrils.

Joseph Orgel and Olga Antipova

Materials for a Sustainable Future



Speakers in Materials for a Sustainable Future. Front: Andrey Yakovenko, Christopher Cahill, Debasis Banerjee, Greg Halder; back: Winnie Wong-Ng, Hong-Cai Zhou, Karena Chapman, Fernando Uribe-Romo.

The symposium provided an overview of neutron and X-ray scattering studies on materials that address key energy-related problems. H.-C. Zhou (Texas A&M) designed and characterized selective metal-organic frameworks (MOFs) for carbon capture. Carbon capture in MOFs was also addressed by D. Banerjee (Rutgers U.) and W. Wong-Ng (NIST). Studies of uranium-bearing hybrid materials relevant to nuclear energy were presented by C. Cahill (George Washington U.), and K. Chapman (ANL) described a MOF-based trap for hazardous by-products of nuclear energy production. F. Uribe-Romo (Cornell U.) presented his work with porous covalent organic frameworks (COFs), including highly ordered COF thin films for organic photovoltaic devices.

S. Chundawat (Michigan State U.) described a biomass-to-biofuel conversion process, an important route to energy sustainability. Anhydrous liquid ammonia pretreatment reorganizes the hydrogen-bonding network in the crystalline structure, giving the biomass improved enzymatic deconstruction efficiency. H. O'Neill (ORNL) discussed development of a biohybrid photoconversion system that combines natural photosynthetic apparatus with synthetic block copolymers to expedite solar energy conversion. M. Everett (ORNL) described neutron powder diffraction studies of seafloor methane hydrates. She suggests that formation of carbon dioxide hydrates could release methane as an energy source and simultaneously reduce carbon dioxide in the environment. J. Cole (U. of Cambridge) quantified structure-property relationships of materials for dye-sensitized solar cells.

N. Chernova [Binghamton U./Northeastern Center for Chemical Energy Storage (NECCES)] studies atomic-scale processes which govern electrode function in rechargeable batteries (EFRC), using pair-distribution function (PDF) analysis, X-ray absorption spectroscopy, electron microscopy, Li NMR and magnetic properties. O. Borkiewicz (ANL/NECCES) examines the spatial evolution of electrochemical reactions and reaction fronts using *in situ* X-ray PDF analysis. C. Bridges (ORNL) described his studies of disorder and defects in Li-ion cathode materials.

Gregory Halder, Sai Venkatesh Pingali and Andrey Yakovenko

Diffraction Studies of Animals, Plants and Insect Bodies



Speakers in Diffraction Studies of Animals, Plants and Insect Bodies. Rama Sashank Madhurapantula, Barbara Brodsky, Dan Kirschmer, Joseph Orgel, Jeff Deschamps, Olga Antipova, Tom Irving, Li-Kai Liu and Simon Goodson.

The session focused on studies of animal, plant and insect connective tissues while they were still principally intact. B. Brodsky (Tufts U.) reviewed the history of collagen studies, from early investigations of its helical symmetry through studies of collagen packing and fibril forms, noting the different methods used over the years. Several of the key investigators in the study of collagen and fibrous elements were present in the audience. Etter Lecturer S. Goodson (Cardiff U.) found agreement between the type I collagen packing structure he found in mouse tissue with that previously reported for rat type I collagen packing structure, a model organism specifically suited to the study of human diabetes. D. Kirschner (Boston College) combined X-ray and neutron diffraction of rodent nerve cells to differentiate between CNS and PNS nerves. The scans of rodent nerves, which showed clear and recognizable myelin diffraction, may lead to routine detection of differences in nerve structure, distinguishing pathological from normal conditions.

Joseph Orgel and Olga Antipova

Complementary Methods



Speakers in Complementary Methods. Jacqueline Cherfils, Christopher Dettmar, Michel Fodje, Julien Cotelesage, Catherine Lawson, Stephen Tomanicik, Shyamosree Bhattacharya, Filip Van Petegem.

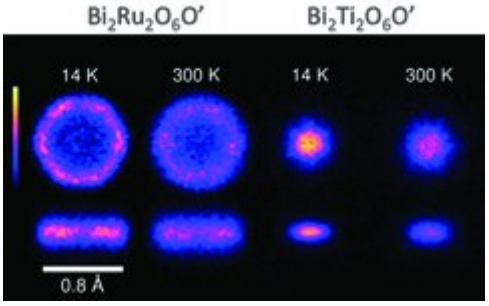
F. Van Petegem (U. British Columbia) combined electron microscopy reconstruction maps and single-crystal X-ray structural models to investigate malignant hyperthermia and cardiac arrhythmias. Comparisons between wild-type and mutant ryanodine receptor models revealed that mutations lead to premature and prolonged opening of the calcium channels, resulting in abnormal calcium release. C. Lawson (Rutgers U.) described the EM Databank, a unified data resource for three-dimensional electron microscopy and a one-stop shop for EM-related data, and the tools for depositing, accessing and visualizing EM-related data. S. Tomanicek (ORNL) described progress with the X-ray structure determination of a metallochaperone-like domain of mercuric reductase (MerA). The MerA structure has two arms with conserved -SH groups, which bind mercury and transfer it to the core for catalysis. J. Cherfils (Centre National de la Recherche Scientifique) described the structure and dynamics of Arf GTPases, important regulators of exo- and endocytocis. A combination of SAXS, NMR, immune-labelling electron microscopy and tryptophan fluorescence revealed structure-based functional differences between Arf1 and Arf6. Etter Lecturer C. Dettmar (Purdue U.) described an instrument for integrating second-order nonlinear imaging of chiral crystals (SONICC) and two-photon excited ultraviolet fluorescence imaging (TPE-UVF) with a synchrotron X-ray diffraction beam line. By combining SONICC and TPE-UVF, the capabilities for imaging tiny crystals with a high depth of field are significantly improved over existing methods. J. Cotelesage (U. Saskatchewan) described how X-ray absorption spectroscopy provides more accurate bond lengths between metals and their ligands than diffraction experiments, as well as information about the oxidation state of metal ligands that is not available from diffraction experiments. He described efforts to integrate online X-ray absorption spectroscopy and diffraction at the Canadian Light Source. S. Bhattacharya (U. Wisconsin-Madison) described how X-ray structure determination of wild-type and mutant phytochrome is guiding protein engineering efforts to design a smaller, more compact and more stable fluorescent phytochrome biomarker.

Michel Fodje

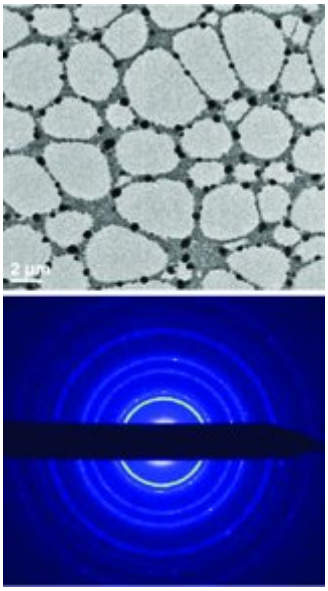
Local Structure and Partially Ordered Systems



Speakers in Local Structure and Partially Ordered Systems. L to R: Branton Campbell, A. M. Abeykoon, Breaunnah Bloomer, Elena Aksel, Daniel Shoemaker, Katharine Page, Mikhail Feygenson and Claire Saunders. (Absent: Co-chair Thomas Proffen.)



Real space maps of static Bi displacements in insulating $Bi_2Ti_2O_6O'$ and metallic $Bi_2Ru_2O_6O'$ are viewed along (top) and normal to (bottom) the O-Bi-O bond. Static disorder in both produces hexagonal ring or disk shapes centered on the ideal position, with striking differences in displacement magnitude. D. P. Shoemaker, R. Seshadri, M. Tachibana and A. L. Hector, 'Incoherent Bi off-centering in $Bi_2Ti_2O_6O$ and $Bi_2Ru_2O_6O$: insulator versus metal', *Phys. Rev. B*, **84**, 064117 (2011).



(Top) A TEM image of ~100 nm Au nanoparticles. Black dots are the nanoparticles on the grid and the large white areas are the holes in the grid. (Middle) A background-subtracted electron diffraction image, collected from the same region of the sample using 200 keV electrons. (Bottom) The one-dimensional electron diffraction pattern obtained by integrating around the diffraction rings. The inset shows a magnified region of the integrated electron diffraction pattern, as indicated by the dotted lines. M. Abeykoon, C. D. Malliakas, P. Juhas, E. S. Bozin, M. G. Kanatzidis and S. J. L. Billinge, 'Quantitative nanostructure characterization using atomic pair distribution functions obtained from laboratory electron microscopes', *Z. Kristallogr.* **227**, 248-256 (2012).

D. Shoemaker (ANL) demonstrated how data-driven reverse Monte Carlo simulations can create large-box models to capture atomic disorder in complex materials while separate constraints (PDF, Bragg, bond valence) can be satisfied simultaneously. Among his examples were complex oxides, crystal growth, and semiconducting chalcogenides. M. Abeykoon (BNL) showed that, using the pair distribution function (PDF), data of sufficient quality for quantitative analysis of nanoparticle structures can be obtained with a transmission electron microscope (TEM). The ease of data collection and ubiquity of TEMs could make this an important tool in the characterization of nanostructured materials if the barriers to data processing can be overcome. B. Campbell (Bringham Young U.) fits local structure models to three-dimensional volumes of single-crystal X-ray diffuse scattering data in relaxor ferroelectrics. He discussed Huang scattering from point defects that produce long-range distortion fields in the surrounding material, which Campbell explained were, 'much like those that troubled the sleep of the princess in the story of The Princess and the Pea' (!). M. Feygenson (ORNL) related how PDF analysis can provide quantitative information about the local arrangement of atoms, enabling studies of defects, surface relaxation and local disorder in nanomaterials. Etter Lecturer E. Aksel (U. of Florida) discussed

local deviations from the average structure of $Na_{0.5}Bi_{0.5}TiO_3$ ferroelectric ceramics. Undergraduate B. Bloomer (LANL/Howard U.) demonstrated local structural changes occurring during geopolymerization synthesis, and undergraduate C. Saunders (ORNL/Duquesne U.) discussed instrument resolution effects on PDFs.

Katharine Page

In situ Parametric Studies



Speakers in *In situ* Parametric Studies. L to R: Antonio dos Santos, Scott Misture, Kamila Wiaderek, Garrett Granroth, Dermot O'Hare, Mario Wriedt, Peter Khalifah. Inset: Xiang-quiang Chu.

D. O'Hare (Oxford U.) has designed a custom-built cell that allows the study of reactions *in situ*, using energy-dispersive and monochromatic X-rays. The flux growth of $Bi_5Ti_3Fe_{(1-x)}Mn_xO_{15}$ Aurivillius phase under different experimental conditions was monitored and it was observed that product formation is preceded by the formation of an intermediate phase. M. Wriedt (Texas A&M) described a copper-based metal-organic framework material containing neutral nitrogen-rich moieties, for which a single reaction led to the formation of three crystal forms of different hydration states. The crystal and hydration states are interchangeable and dependent on temperature and humidity, and water content alters magnetic properties. G. Granroth (ORNL) used the Sequoia time-of-flight spectrometer at the Spallation Neutron Source to determine the magnetic structures of two high-field magnetic phases of $MnWO_4$, a multiferroic material with a magnetic phase diagram of at least six phases.

S. Misture (Alfred U.) described *in situ* studies of transition metal oxides with potential applications in fuel cells. Electrochemical activity was monitored at high temperatures and under controlled atmosphere, mimicking the operation environment of fuel cells. P. Khalifah (SUNY Stony Brook) discussed degradation of $LiFeBO_3$, a high-capacity battery material. The crystal structure was redetermined based on a four-dimensional modulated space group $C2/c(1/200)00$. It was found that modulation hindered Li mobility and that the performance of $LiFeBO_3$ can be improved by reducing this modulation. K. Wiaderek (ANL) studied the structure and size of nanoparticles in iron-based battery materials under operational conditions. A ripening of the nanoparticles observed upon cycling may contribute to observed performance degradation.

X.-Q. Chu (ORNL) discussed the use of quasi-elastic neutron scattering to study the relaxational dynamics of hen egg white lysozyme and an inorganic pyrophosphatase. The slow dynamics of these globular proteins could be adequately modeled by the mode-coupling theory that predicts a logarithmic decay of the relaxation time.

Antonio dos Santos

From Constructs to Crystals



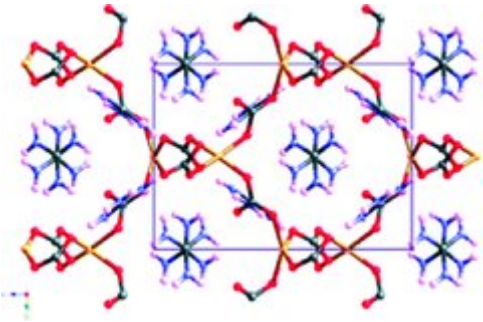
Speakers in From Constructs to Crystals. Front: Eric Ortland, Zygmunt Derewenda, David Waugh and Miki Senda; Glen Spraggon, Todd Green, Nicholas Noimaj, Patrick Shaw Stewart and George Lountos.
This session addressed membrane protein expression, purification and crystallization (N. Noinaj, NIDDK / NIH), using the maltose binding protein as a fusion partner which has become a staple of protein purification (D. Waugh, NCI), the ins-and-outs of protein and nucleic acid production and crystallization (T. Green, U. Alabama), and enhancing the crystallizability of proteins *via* surface entropy reduction (Z. Derewenda, U. Virginia). Noted that replacing bulky hydrophobic residues with alanine may improve protein solubility and stability.

Eric Ortlund and George Lountos

Functional Materials and Technology



Speakers in Functional Materials and Technology. Front: Elinor Spencer, Margot Fabian, Craig Bridges, and James Kaduk; back Emil Bozin, Tiffany Kinnibrugh, Hans-Conrad zur Loye, and Andrey Yakovenko. (Max Kaganyuk not shown.)



The high-pressure behaviour of the three-dimensional copper carbonate framework $\{[Cu(CO_3)_2](CH_6N_3)_2\}_n$ by Elinor C. Spencer, Nancy L. Ross and Ross J. Angel, *J. Mater. Chem.* (2012), **22**, 2074-2080, DOI: 10.1039/C2JM15206A, published online Dec. 2011.
The session began by looking at inorganic solids synthesized using high-temperature (fluxes) or hydrothermal (supercritical water) solvents. H. zur Loye (U. South Carolina) showed that metal hydroxides are very effective for the growth of high-quality mixed metal oxide single crystals. E. Bozin (BNL) showed by PDF techniques that Ir^{4+} dimers exist locally in $Cu(Ir_{1-x}Cr_x)_2S_4$, even though long-range order is absent.

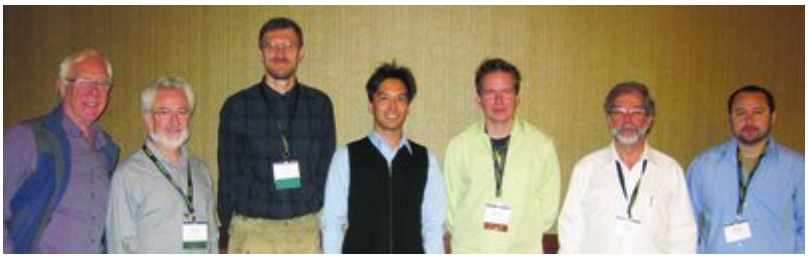
With high-pressure single-crystal studies, E. Spencer (Virgina Tech) showed that three-dimensional metal-organic hybrid materials can be as strong as zeolites.

T. Kinnibrugh (Texas A&M) used powder diffraction techniques to characterize the structural changes on dehydration of potentially nanoporous Zn phosphonate compounds. Combining X-ray and neutron PDF measurements and reverse Monte Carlo simulations, M. Fabian (LANL) showed that the glassy networks in MoO_3-Bi_2O_3-WO_3 systems are built up of distorted MoO_4 tetrahedra and mixed WO_3/WO_4 or BO_3/BO_4 structural units.

A. Yakovenko (Texas A&M) showed that structure envelope density maps can be used to determine the pore structure and locations of guest molecules in MOFs.

James A. Kaduk & Craig Bridges

Membrane Proteins: Start to Finish



Speakers in Membrane Proteins: Start to Finish. Robert Stroud, Robert Fischetti, Vadim Cherezov, Eugene Chun, Tommi Kajander, Ehud Landau, and Nicholas Noinaj.
Membrane proteins that perform essential cellular functions are major drug targets and challenging candidates for structural analysis. Financial support for major initiatives has produced exciting structures of ion channels, G protein-coupled receptors, transporters and other membrane protein families. This session was devoted to persistent challenges in this important field. R. Stroud (UCSF) discussed expression systems for production of eukaryotic membrane proteins and his structure determination of components of a zinc pump belonging to a superfamily of membrane proteins.

About 15 years ago, E. Landau (U. of Zürich) and J. Rosenbusch (Biozentrum) began crystallizing membrane proteins using a greasy lipidic mesophase known as lipidic cubic phase (LCP). At the time, some considered this method to be revolutionizing, while others believing it would be a 'one-trick pony', suitable only for a specific class of proteins. The LCP crystallization method has contributed more than 100 membrane protein structures to the PDB, including 32 proteins from at least seven different families, including the highly challenging superfamily of G protein-coupled receptors. While it takes an effort to perfect LCP technologies, labs that took the plunge have been highly successful and the perspectives look bright for newcomers.

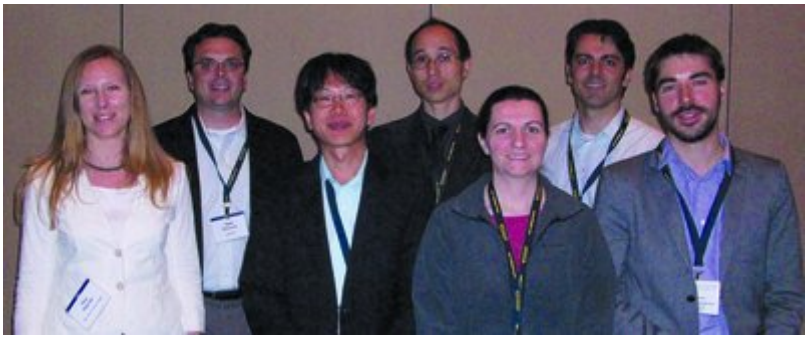
N. Noinaj (NIDDK) talked about nits and grits of his work on structural determination of components of a β-barrel assembly complex. Significant progress has been made during the last few years at synchrotron beamlines, allowing for data collection on ever smaller crystals of more challenging targets. R. Fischetti (GM/CA CAT, APS) described instrument developments of particular relevance to studies of membrane proteins, including a SONICC system for detection and alignment of optically invisible small crystals.

Etter Student Lecturer E. Chun (Scripps Research Inst.) developed a fusion partners toolchest for stabilization and crystallization of G protein-coupled receptors (GPCR). Chun described in detail the procedures followed to identify a fusion partner that would cocrystallize with GPCR and yield the best structure to date of a GPCR (1.8 Å resolution), The same fusion partner was used to determine a structure of the nociceptin/orphanin FQ opioid receptor.

T. Kajander (U. of Helsinki) described his studies of Na-pumping pyrophosphatase from Thermotoga maritima at 2.6 Å resolution in a resting state and with a bound product that shed light on the sodium pumping mechanism and suggested that the protein has evolved through gene triplication. The session including reports on the details of the structure determinations of five new membrane proteins was supported by contributions from Avanti Polar Lipids and TTP LabTech.

Vadim Cherezov

Pharmaceutical Research and Development



Speakers in Pharmaceutical Research and Development. Noa Marom, Matthew Peterson, Eugene Cheung, Eric Chan, Magali Hickey, Mark Oliveira, and Peter Wood. (Patrick Connelly not shown.)
P. Connelly (Vertex Pharmaceuticals) showed examples of combining crystallographic, computational and thermodynamic data to guide drug design. P. Wood (CCDC) presented an assessment of isostructurality in pharmaceutical salts, highlighting the lack of similarity and predictability between crystal structures of most sodium and potassium salts of drug-like molecules. E. Cheung (Amgen) illustrated the differences between thermal expansion, dehydration and form change using variable-temperature powder diffraction data. N. Marom (U. Texas, Austin) described advances in dispersion correction schemes employed in DFT computations, with case studies on several polymorphic systems. E. Chan (Bristol Meyers Squibb) discussed models of the diffuse scattering from single crystals of two aspirin polymorphs, highlighting the power of the diffuse scattering method in comparison to routine analysis of diffraction data. M. Oliveira (Alkermes) described the structure of an opioid modulator and a structural and computational analysis of closely related analogs.

Matthew Peterson and Magali Hickey

Structure-Guided Drug Discovery



Speakers in Structure-Guided Drug Discovery. Front: Jaeok Park, Helen Berman, Shraddha Thakkar and Stephen Burley; back: Stefan Knapp, Gregg Crichlow, Alan Hruza, David Eisenberg.

S. Knapp (Oxford U./Structural Genomics Consortium) presented studies targeting epigenetic effecter domains of the bromodomain family. H. Berman (Rutgers U./PDB) described advances in data management of small molecule ligands, antibiotics and peptide inhibitors in the PDB. D. Eisenberg (UCLA) presented efforts to find small-molecule inhibitors of amyloid formation. A. Hruza (Merck Research Laboratory) explained how modest resolution X-ray structures of the aurora kinase catalytic domain allowed structure-based design of imidazo[1,2-*a*]pyrazine inhibitors.

Etter Lecturer S. Thakkar (U. of Arkansas) discussed her structure-based design of anti-methamphetamine single-chain antibodies.

Stephan Burley

Data Collection with the Pros



Speakers in Data Collection with the Pros. Andrew Torelli, Edward Collins, Zbigniew Dauter, James Holton and Raj Rajashankar.

The 'Blackboard' sessions at this year's meeting focused on best practices for data collection and included a real-time demonstration of data collection on SER-CAT's ID beam line at ANL (Z. Dauter, NCI), a discussion of critical sources of error found in crystallographic data that can make the difference between solvable and intractable data led by J. Holton (UCSF/BMB/PBD) and instruction on collecting data using the six million detectors that comprise the latest PILATUS X-ray detector arrays (R. Rajashankar, Cornell U.). Links to the Powerpoint slides and videos of the talks can be found on the ACA website. Click on the 'Jobs/Education' link at the top of the ACA home page and then click on the 'Blackboard Sessions' link under the 'A Crystallographer's Resources' section heading. Next year's Blackboard session will address structural validation.

Andrew Torelli and Ed Collins

Inorganic Phase Transitions



Speakers in Inorganic Phase Transitions: Stacey Smith, Marcus Bond, Elinor Spencer, Mario Bieringer, Patrick Mercier, Branton Campbell and Saurabh Tripathi.

P. Mercier (NRC, Canada) presented a systematic analysis of the layer-stacking polytypes available within the kaolin system. *Ab initio* DFT calculations of the energy and enthalpy of each polytype make it possible to rationalize the experimental phase sequence observed up to 60 GPa. E. Spencer (Virginia Tech.) discussed supercells, symmetries, superlattice reflections, volume changes and group-subgroup relationships in two high-pressure phases of the mineral petalite ($LiAlSi_4O_{10}$). S. Smith (Brigham Young U.) described two types of high-temperature surface area loss, the location of the La atoms in La-doped gamma-alumina nanoparticles and a potential mechanism for the La-stabilization of the gamma phase. M. Bieringer (U. of Manitoba) described phases in the $Sc_{1-x}Lu_xVO_3$ perovskite family. He found that the smaller Sc cation results in a disordered bixbyite structure, while the larger Lu cation results in a perovskite phase. High-pressure stabilization of the Sc-rich perovskite phases made it possible to track the physical properties of the family across the boundary between stability and metastability. S. Tripathi (Central Michigan U.) discussed particle size influence on the ferroelectric polarization of $YMnO_3$. M. Bond (SE Missouri State U.) explained that, due to strong ligand-ligand interactions, it was concluded that $CuBr^{4-}$ salts were incapable of forming the square-planar complex observed in some $CuCl^{4-}$ salts. However, a square-planar to flattened-tetrahedral transformation has now been observed in 1,2,6-trimethylpyridinium salts of both $CuCl^{4-}$ and $CuBr^{4-}$.

Branton Campbell

MISCELLANY

My Favorite Crystal



The Belgian National Committee for Crystallography has organized since 2000 a national crystal growing competition for pupils in the secondary schools (ages 12-17 years). During a period of five weeks the pupils should grow single crystals of a compound that is sent to the registered schools by one of our sponsors. On the website of the competition more information is given on crystals in general, the compound to crystallize and how to grow single specimens. The pupils are of course guided by their science teacher and in case of problems they can contact a local member of the national committee. A jury judges the quality of the crystals based on their mass, transparency, faces *etc*... Each year I am surprised at the quality of the submitted crystals, which makes the judging of more than 200 crystals not an easy task! So it is with pleasure that I nominate one of the prize-winning crystals from a previous edition as my favorite crystal! The crystal shown here is a beautiful alum crystal crystallized by a group of three 15 year-old pupils of the Athénée Royal de Bruxelles II during the edition 2007. The size is about 2 cm and the quality is almost perfect!

Many countries have similar crystal growing competitions, so IYCr2014 is the perfect time to organize a World Crystal Growing Competition to bring as many young people as possible in contact with our fascinating world of crystals!

Luc Van Meervelt

MEETING REPORT

Seventh Belgian Symposium

Brussels, Belgium, October 2012
www.chem.kuleuven.be/bcc/bcs/



Speakers at the Seventh Belgian Crystallography Symposium BCS-7. Andrew Thompson, Yaroslav Filinchuk and Elias Vlieg.

More than 80 scientists took part in the Seventh Belgian Crystallography Symposium, BCS-7, which was held on October 10, 2012, at the Academy House, adjacent to the Royal Palace in Brussels, under the aegis of the Belgian National Committee for Crystallography. Due to the success of previous BCS meetings, the National Committee for Crystallography organizes this symposium at biennial intervals to promote contacts between Belgian scientists using diffraction and microscopy techniques for studies in the fields of condensed matter chemistry and physics, materials sciences, earth sciences and life sciences. As one of the main objectives was to promote personal contacts, plenary lectures were limited to three and given by distinguished colleagues in widely different fields.

During the opening lecture by Andrew Thompson (Gif-sur-Yvette), a nice overview was given of the use of synchrotron radiation in the case where one has tiny crystals or tiny anomalous signals. The macromolecular crystallography beamline PROXIMA 1 at SOLEIL uses hereby the flexibility of the multi-axis geometry. Complex hydrides such as bimetallic borohydrides are the favorite study materials of Yaroslav Filinchuk (Louvain-la-Neuve). These materials can be used for hydrogen storage and their structure and reactivity are studied mainly by *in situ* powder diffraction. The morning session was closed by Elias Vlieg (Nijmegen) with a talk on crystal growth. Examples in the field of nanowires and high-quality protein crystals were shown, as well as the use of grinding techniques to convert racemic mixtures into chirally pure compounds.

A poster session and commercial exhibition was organized during lunchtime. For the afternoon session, three oral presentations were selected from the submitted abstracts (Cedric Gommes, Liège; Senne Van Rompaey, Antwerp; Neil Brooks, Leuven). Two poster prizes were awarded, to Maria Batuk (Antwerp) and Stephen Weeks (Leuven). The meeting was sponsored by the Royal Academies of Sciences and Art of Belgium, and by the firms Agilent, Bruker AXS, FEI Europe, STOE, Sysmex and Xenocs.

Luc Van Meervelt

AWARDS AND PRIZES

2012 Chemistry Nobel to Lefkowitz and Kobilka



Robert Lefkowitz



Brian Kobilka

Robert Lefkowitz and Brian Kobilka shared the 2012 Nobel Prize in Chemistry for groundbreaking discoveries that revealed the inner workings of G-protein–coupled receptors (GPCRs), a large family of membrane-bound recepters that influence most aspects of our health and are prime targets for drug action. In 1968 Robert Lefkowitz labeled various hormones with radioactive iodine in order to identify receptors that bound the hormones, including the receptor for adrenalin. He extracted the receptor from the cell wall and gained an initial understanding of how it works.



Crystal structure of activated β-2 adrenergic receptor β2AR (red) in complex with G-proteins (green, cyan and yellow). Credit: S. G. F. Rasmussen *et al.*, Nature, **477**, 549–555 (2011).

In the 1980s, Brian Kobilka isolated the gene that codes for the β-adrenergic receptor from the human genome. The team realized that this receptor looked very similar to the rhodopsin receptor from the eye. They realized that there is a whole family of GPCRs that look alike and function in the same manner. The studies by Lefkowitz and Kobilka are crucial for understanding how GPCRs function because about half of all medications achieve their effect through GPCRs. In 2011, Kobilka and his research team captured an image of the β-adrenergic receptor at the exact moment that it is activated by a hormone and sends a signal into the cell. This image is a molecular masterpiece – the result of decades of research.

From ACA RefleXions, Winter 2012

REGIONAL NEWS

Fortier chosen as McGill’s new Principal and Vice-Chancellor



Suzanne Fortier was chosen to be McGill’s new Principal and Vice-Chancellor, effective September 2013. The decision was recently made public after a months-long search. Fortier will replace Heather Munroe-Blum, who has been leading the University since 2003, and who will be stepping down June 30, 2013. An Acting Principal will be appointed to serve from July until September. Fortier, a McGill alumna, has been serving since 2006 as the president for the Natural Sciences and Engineering Research Council of Canada (NSERC), a government agency that provides research grants in the natural sciences and engineering fields.

REGIONAL NEWS

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OBITUARY

Louise Napier Johnson (1940-2012)



Louise Johnson, biophysicist and structural biologist, died after a 13-month illness which she bore with quiet fortitude and grace. Her life and work impacted very many people worldwide, due to her scientific activities in protein crystallography and enzymology, and her tireless interest and effort in supporting and encouraging scientists in developing countries to establish effective research laboratories as far apart as South America, the Middle East and Pakistan. I am one of those whose life course was changed by Louise.

In the early 1980s her group at Daresbury Laboratory near Runcorn was in the vanguard of those using synchrotron radiation for macromolecular crystallography. Louise’s lifelong interest in applying new techniques to structural biology questions came to the fore when she became Life Sciences Director of Diamond Light Source in 2003. There she oversaw the building and development of this highly effective national facility which is now bearing great fruit for the UK physical and biological sciences research community.

I went to work with Louise when she was appointed to the David Phillips Chair in Molecular Biophysics in 1990. Her management style was 'hands off' but 'attention on' in that she was always there if advice or guidance was needed. Although Louise did not normally accompany us on trips to the synchrotron, during one of her sabbatical terms she worked her way through our usual training program for new researchers, asking penetrating and pertinent questions at every stage. This was a great example to us of how a senior scientist should keep in touch with what daily research really involved, so that challenges faced by students and postdocs could then be better appreciated and overcome.

Her book written with Tom Blundell is a classic text in the field. Her last book with W. Baumeister, A. C. Steven and R. Perham, *Molecular Biology of Machines and Assemblies*, will be published this year. Along with her numerous colleagues throughout the world, I will miss her inspiration scientifically and personally. I was privileged indeed to have known and worked with her.

Elspeth Garman, ACA RefleXions, Winter 2012

OBITUARY

Boris Kamenar (1929 – 2012)



Boris Kamenar, a fellow of the Croatian Academy of Sciences and Arts (CASA), and internationally recognized scientist, passed away in Premantura, Croatia, on July 12, 2012. He was a dedicated teacher of inorganic chemistry and crystallography and supervised thirty MSc and PhD students at U. of Zagreb. He was President of the Croatian Chemical Society of Yugoslavia (1976–1980), Sec. of the Yugoslav Centre of Crystallography (1966–1990), Pres. of the Croatian Crystallographic Association (1991–2005), and Vice-President and President of the European Crystallographic Committee (1978–1984). He was the representative of CASA on the Governing Board of the European Science Foundation and Pres. of the Board for international collaboration of CASA. He was a member of World Academy of Sciences and Arts and of the Macedonian Academy of Sciences and Arts. He received the Ruđer Bošković Award, the State Award for Lifetime Achievements, the Božo Težak Medal and the Medal of the Chemistry Department, Zagreb.

Kamenar was born on Feb. 20, 1929 in Sušak (now Rijeka).He graduated in chemical technology at the U. of Zagreb and established the Laboratory for Chemical and Mechanical Investigations at The Cranes Factory and Foundry, Vulkan, in Rijeka. In 1956 he joined Drago Grdenić at the Ruđer Bošković Institute in Zagreb working on silicon and boron chemistry.

In 1960 he defended his thesis *A new method for obtaining pure silicon and boron* at U. of Zagreb and then taught there until he became professor emeritus in 2000.

B. Kamenar did postdoctoral research with Dorothy C. Hodgkin in Oxford (1964/65) where he was later a Visiting Fellow (1971/72). He was also a visiting professor at U. of New Zealand. His scientific interest was X-ray structural analysis of inorganic, coordination and organometallic compounds, and compounds of pharmacological importance. His first structural studies concerned tin(II), arsenic(III) and antimony(III) compounds that confirmed that the Sidgwick-Powell rule could be applied to heavy atoms. In 1973 he published *Crystal Structures of Electron-Donor-Acceptor Complexes*, a review article written with K. Prout in the book *Molecular Complexes* (edited by R. Foster). His review article on iron complexes written with Branko Kaitner appeared in *Structural Studies on Molecules of Biological Interest*, a volume dedicated to Dorothy Hodgkin. He studied molybdenum complexes and polyoxomolybdates, as models of enzymes as well as catalysts. He investigated molecules of biological and pharmacological importance including intermediates in corrin synthesis, macrocyclic antibiotics and potential antihyperglycemics during his long-term collaboration with the PLIVA Pharmaceutical Company. He determined the structure of an histamine H2-receptor antagonist in collaboration with Smith, Klein and French Laboratories Ltd.

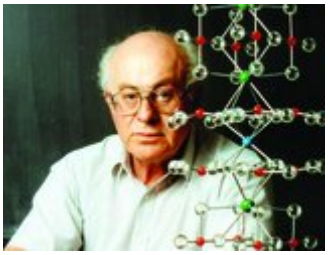
He published over 160 scientific papers, many of them in textbooks and monographs. He chaired or co-chaired many national and international conferences, committees and symposia.

Boris Kamenar’s many friends, colleagues and co-workers will miss his powerful, pleasant and optimistic personality.

Marina Cindrić, Zagreb

OBITUARY

Hugo Steinfink 1924 – 2012



Hugo Steinfink, past president of the ACA and professor emeritus in chemical engineering at U. of Texas at Austin, passed away at the age of 88, on August 25th, 2012, following complications from a cardiac procedure. Born in Vienna, Austria on May 22, 1924, Hugo arrived in New York City in 1939. In 1941, he entered City College of NY, but World War II interrupted his studies when he served as an Army medic. He received a BS in chemistry in 1947, followed by a master's degree in 1948 from Columbia U. When Hugo began work at Shell Development Company, he was assigned responsibilities for the X-ray diffraction laboratory. He talked his boss into letting him attend one of Isidor Fankuchen's 'Two Week Wonders' short courses. He returned to Fan's lab in New York in 1952, where he earned his PhD in X-ray crystallography at Brooklyn Polytechnic Inst. With Fan, Ben Post and Josh Ladell, Hugo developed a low-temperature Weissenberg camera and used it to determine the structure of octamethyl cyclotetrasiloxane, an important monomer in the production of silicone polymers.

He returned to Shell in Houston where he specialized in silicate mineral and organo-silicon crystal structures. He was made Fellow of the Mineralogical Society of America in 1956 and was listed in American Men and Women of Science, Who's Who in Technology, and Who's Who in the South and Southwest. In 1960 Hugo left Shell Development for a career at U. of Texas at Austin, helping to build its 'ceramics' programs. A 1962 Time magazine reported that Steinfink was brought to Texas with the promise of unlimited freedom and a $30,000 diffractometer. The presence of Steinfink and a new, $4,000,000, eight-story laboratory were used to lure U. of Illinois' chemist William Bradley, a leading authority on the molecular structure of materials, to Texas. Hugo was appointed the Jewel McAlister Smith Prof. in Engineering in 1981, and named the T. Brockett Hudson Prof. of Chemical Eng. He was a co-initiator of the Materials Science and Engineering Graduate Program of UT that became a PhD degree granting program. Hugo loved teaching X-ray crystallography. In the 1970s he resurrected Fan's Two Week Wonders by teaching a one week complete course in powder diffraction.

Hugo authored and co-authored over 150 technical publications concerning structure-property relationships in solid-state materials (silicates, zeolites, chalcogenides and high-temperature superconductors). Along with Steve Swinnea he determined the structure of a basic superconductor just before the start of the 1987 ACA meeting in Austin. An evening session presenting the same results was added to the program two days before the 'Woodstock of Physics' session at the New York APS meeting. In his last months Hugo was working with colleagues on a novel cubo-siloxane structure.

He was a member of the American Institute of Chemical Engineers, Phi Beta Kappa, Phi Lambda Upsilon, and Sigma Xi. He was Chairman of the American Chemical Society, Central Texas Section (1966), served on the USNCCr, was President of the ACA (1995), a co-editor of *Acta Crystallographica* (1984-93) and an Associate Editor of *American Mineralogist* (1970-72). He was a board member of the American Inst. of Physics (1989-95) and a visiting professor at the U. of Lille, France (1995).

Hugo was a patient and giving man who combined his brilliance, sense of fairness and curiosity with a dry wit. He shared his life experiences from his childhood in Nazi Vienna to the latest books he thought worthwhile for all to read. He instilled his thirst for knowledge in his children and grandchildren.

Hugo was an avid tennis and squash player most of his life. He traveled the world, including a safari in Africa for his 80th birthday. He was devoted to Cele, his adoring wife of 64 years. He was loved and respected by his family, and many friends, colleagues and students.

ACA RefleXions, Winter 2012

OBITUARY

Guy Dodson FRS (1937-2012)



One of the most beloved and influential figures in the development of protein crystallography, Guy Dodson passed away peacefully on Christmas Eve, with his wife Eleanor and other family members at his side. Guy was an inspirational scientist whose engaging personality and passion for science have enriched the lives of many people round the world. I consider it a personal privilege to have known him.

Guy was born in Palmerston North, New Zealand, a small provincial city he liked to describe affectionately as 'the centre of the universe'. His secondary education was at a small Auckland school with a mission to 'support, educate and train' boys from disadvantaged backgrounds. Whether Guy was ever 'trained' is debatable but there he and his twin brother Maurice acquired a love of sport, history and science, together with a healthy disregard for authority. Guy's love of crystallography and the concept of 'seeing molecules' came as a student at the Auckland University College. He found there an excellent crystallography research group, and undertook the X-ray analysis of a plant alkaloid for his PhD. He remained very grateful for the freedom given by his tolerant supervisor, David Hall, who gave guidance, support and crystallographic training while turning a blind eye to the impromptu cricket, water fights, fire extinguisher episodes etc. that punctuated laboratory activities.

Guy moved to Oxford in 1962 for postdoctoral studies with Dorothy Hodgkin. This move transformed his life. He became Dorothy's right-hand person in the successful solution of the structure of insulin, achieved in 1969, he met and married Eleanor, and he fully embraced the Hodgkin philosophy of allowing individual talent to mature. I came to Oxford in 1967, where I, in turn, became absorbed into the insulin team, socially and scientifically. Guy and Dorothy shaped my whole approach to science, making me feel that it was important, exciting and fun, and best of all that I could do it! I went back to New Zealand full of confidence.

Guy remained in Oxford until 1976 when Dorothy retired. Guy was sometimes asked 'what will you do next?' His answer was 'I haven't finished with insulin yet - there are so many interesting variations to explore'. This determination to understand insulin's conformational flexibility and complex biology has been richly vindicated: several billion-dollar drugs in the form of both rapid-acting and long-lasting insulin derivatives, developed by Novo Nordisk in collaboration with Guy's group; and most recently a *Nature* paper on the insulin:insulin receptor structure, where Marek Brzozowski has sustained the York passion for understanding insulin, in collaboration with Colin Ward and Mike Lawrence in Australia. This latter paper, accepted just before Guy's death, brought enormous and very fitting satisfaction.

In 1976 Guy and Eleanor moved to York to set up a new laboratory in the Chemistry Department. Their warmth of personality and large network of friends brought a steady stream of visitors, many of whom found a place in their cavernous home. You never knew who would appear for breakfast. When I arrived with my wife Heather and our family to spend a year (1977-78) in York, the laboratory was very small, just three people. In New Zealand I had solved the structure of a cysteine protease, actinidin, and Guy suggested this as a perfect vehicle for attempting to refine a protein structure from scratch by least

squares. Eleanor's genius for crystallographic methods, which led to her later becoming the central figure in the CCP4 initiative, made it possible, and I was the beneficiary - it was a turning point in my career. I remember vividly the Saturday when we realized the refinement was working, sitting in York Minster listening to Handel's Messiah and thinking about the *R* factor dropping 10%.

Guy's enthusiasm and openness, his generosity of spirit, and his willingness to devote his time to assisting and advising others, similarly attracted many more researchers to the York laboratory, making it a powerhouse in structural biology. Some stayed, to establish their own research programs, others moved on and made outstanding careers elsewhere. Thinking about how the York lab grew, it is clear that Guy was ambitious for good science, but not necessarily to do it all himself; he was very happy to foster and enjoy the efforts of others.

As Dorothy Hodgkin had also done, Guy established effective collaborations with industry, on protein engineering, insulin derivatives and industrially useful enzymes. In 1993, he was persuaded to also lead a Division at NIMR in Mill Hill, where his energies established yet another internationally leading research group, bringing structural insights to biomedical research. He went on to play a major role in research projects dealing with malaria, TB and the structure of prions. Guy had a broad vision. He conducted insightful studies of the mechanisms of action of hemoglobin and a variety of hydrolytic enzymes: penicillin acylases, amylases and lipases. His greatest delight came as he explored the exquisite beauty of catalytic sites, perfectly oriented hydrogen bonds and strategically placed water molecules.

As Chair of the IUCr Commission on Biological Molecules he led the way in establishing criteria for the deposition and release of both the data and the coordinates for biological structures, driven by the belief that they should be available to all. He campaigned tirelessly on issues such as the location of the Diamond Synchrotron and the NIMR. His wisdom and lack of personal agendas saw him widely sought as a reviewer and a PhD examiner. He had very high standards, but he understood human fallibilities.

Guy liked to say that he had never grown up, and there is some truth in this. He retained a boyish enthusiasm, and his love of life was infectious. He could be describing the exquisite beauty of the catalytic triad in serine hydrolases one moment and be bowling tricky leg-spinners down the laboratory corridor the next. A typical comment from a young researcher in my laboratory sums up his personal legacy: 'Though I met him only a few times I was always struck by his passion for both life in general and science in particular, as well as what I saw as a mischievous twinkle in his eye and his approachableness. I always came away from talking to him with renewed enthusiasm'.

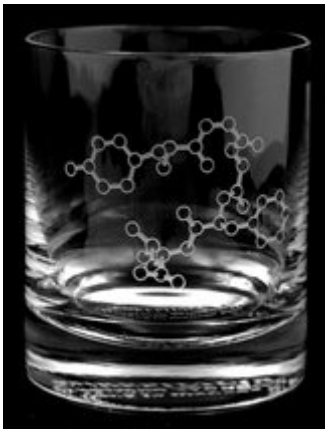
Guy always saw the best in people, and as a result he got the best from them. Today, researchers all round the world, from the UK and Europe, to North America, Cuba, India, China, Australia and New Zealand, carry the benefits of their associations with Guy and an abiding and affectionate love for him.

The full obituary appears in *Acta Cryst.* (2013). D**69**, 490-492.

E. N. Baker

EDITORIAL

From the editor's desk



The cover of this issue highlights the annual meetings of the three regional affiliates of the IUCr where the most recent, reliable and exciting structural chemistry, biochemistry and materials science will be reported months before it will appear in *Science*, *Nature* and leading primary journals in the field. Join the excitement at the meeting closest to you or travel to England, Hawaii or Hong Kong to meet old friends in a new part of the world. The beautiful mineral crystals on the cover are from countries of the three regional affiliates. The images are taken from the book *Color Treasury of Crystals* with text by Vincenzo DeMichele of the Natural History Museum of Milan, published by Instituto Geografico De Agostini in 1972 with the translation published by Orbis Publishing Ltd, London, in 1979. The book contains a brief discussion of crystal systems illustrated with mineral examples of each crystal system. The calcite from Cumberland, England, is triclinic, the twinned quartz crystal from Otomezaka, Japan, is trigonal, and the tetragonal wulfenite from Arizona shows tetrad symmetry. Crystallography has been used to characterize minerals for centuries and the book stresses the enormous variety and beauty of the minerals on earth. I was pleased to rediscover the book on the eve of the International Year of Crystallography.

In this issue IUCr President, Gautam Desiraju, has offered his candidate for a very important crystal, selected by him in part due to its connection to India. Luc Van Meervelt has also offered his choice of an important crystal.

I repeat my invitation to all readers of the *IUCr newsletter* to identify a crystal that is important to you for any reason and write a paragraph explaining why it matters to you, to crystallography, to science or to mankind. A picture of the crystal of your choice would be appreciated but is not essential. The names of those who send in suggestions in the next three months will be put in a hat. A name will be drawn from the hat and Abino Mills Glassworks of Buffalo will prepare four glass mugs with an etching of the structure in the crystal of your choice for the winner.

William L. Duax