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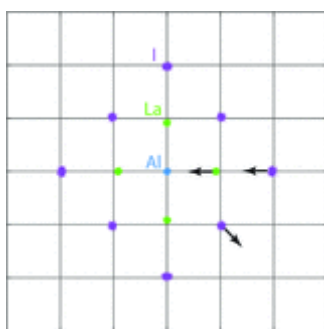
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Reliability of Monte Carlo simulations of disordered structures optimized with evolutionary algorithms exemplified with diffuse scattering from $\text{La}_{0.70(1)}(\text{Al}_{0.14(1)}\text{I}_{0.86(1)})$

Reliability of Monte Carlo simulations of disordered structures optimized with evolutionary algorithms exemplified with diffuse scattering from $\text{La}_{0.70(1)}(\text{Al}_{0.14(1)}\text{I}_{0.86(1)})$

Acta Cryst. (2008). A64, 641-653 (doi.org/10.1107/S0108767308026184)



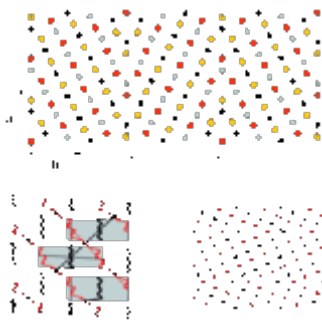
Local relaxations within an isolated $\text{AlLa}_6\text{I}_{12}$ cluster

Complex disorder and corresponding diffuse scattering from the compound $\text{La}_{0.70(1)}(\text{Al}_{0.14(1)}\text{I}_{0.86(1)})$ was taken as the basis for investigating the reliability, reproducibility and influence of refinement parameters of evolutionary algorithm refinements of Monte Carlo simulations. Using the same diffuse scattering data set, a model relying on reasonable a priori knowledge about the real structure was used, as well as one that includes no presumptions except the average structure and the chemical composition. To strengthen the complementary character of the approaches, two different evolutionary algorithms were employed.

T. Weber, A. Simon, H. Mattausch, L. Kienle and O. Oeckler

Modular crystals as modulated structures: the case of the lillianite homologous series

Acta Cryst. (2008). B64, 684-701 (doi.org/10.1107/S0108768108031492)



(x, y) projection of the heyrovskyite structure (a), and continuous functions in superspace representing the x (b) and y (c) coordinates of the atoms in (a). Red (yellow) color represents S atoms at $z = 0$ ($1/2$) and black (gray) color represents Pb/Bi atoms at $z = 0$ ($1/2$).

Modular crystals, such as the heyrovskyite phase in the figure, consist of alternate stacking of two symmetry-related modules with internal approximate subperiodicity. Using the superspace formalism, originally developed for incommensurately modulated crystals, a whole series of commensurate modular structures can be described with atomic modulation functions almost independent of composition and given by few parameters. This superspace approach, with the remarkable zigzag form of the x component of the modulation functions, reveals an underlying misfit between different latent periodicities of cations and anions.

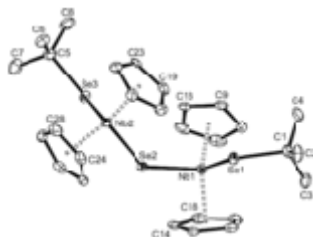
L. Elcoro, J. M. Perez-Mato, K. Friese, V. Petříček, T. Balic-Zunic and L. A. Olsen

IUCR JOURNALS NEWS

[{Cp₂(*t*BuSe)Nb}₂E] (E = O and Se) with bridging oxide or selenide ligands

[{Cp₂(*t*BuSe)Nb}₂E] (E = O and Se) with bridging oxide or selenide ligands

Acta Cryst. (2008). C64, m321-m323 (doi.org/10.1107/S0108270108025055)

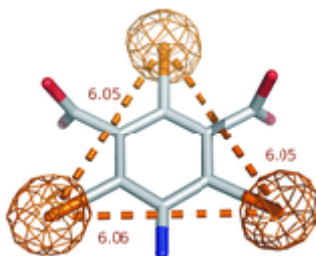


Two dinuclear, oxide- or selenide-bridged, niobium(IV) bis(cyclopentadienyl) *tert*-butylselenolates have been obtained. These are the first organometallic niobium selenolates to be structurally characterised. In the oxide, the O atom lies on an inversion centre and the Nb-O-Nb linkage is linear, whereas in the selenide (see figure) the Nb-Se-Nb angle is 139.76 Å. This difference can be attributed to π bonding in the oxide.

A. L. Hector, M. Jura, W. Levason, G. Reid, S. D. Reid and M. Webster

A magic triangle for experimental phasing of macromolecules

Acta Cryst. (2008). D64, 1179-1182 (doi.org/10.1107/S0907444908030266)



The magic triangle 5-amino-2,4,6-triiodoisophthalic acid (I3C) with three iodine atoms for anomalous scattering, arranged in an equilateral triangle (distances in Å), and three functional groups for hydrogen bonding.

Obtaining phase information for the solution of macromolecular structures is still one of the bottlenecks in X-ray crystallography. The compound 5-amino-2,4,6-triiodoisophthalic acid (I3C) is a representative of a novel class of compounds for heavy-atom derivatization that combines heavy atoms with functional groups for binding to proteins. I3C was incorporated into proteins in order to obtain phases by single-wavelength anomalous dispersion (SAD). An improved binding capability compared with simple heavy-metal ions, improved recognition of potential heavy-atom sites and low toxicity make I3C particularly suitable for experimental phasing.

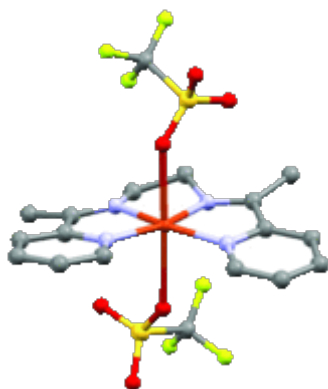
T. Beck, A. Krasauskas, T. Gruene and G.M. Sheldrick

IUCR JOURNALS NEWS

**{N,N'-Bis[1-(2-pyridyl)ethylidene]ethane-1,2-diamine- κ^4 N,N',N'',N'''}
bis(trifluoromethanesulfonato- κ O)copper(II)}**

**{N,N'-Bis[1-(2-pyridyl)ethylidene]ethane-1,2-diamine- κ^4 N,N',N'',N'''}
bis(trifluoromethanesulfonato- κ O)copper(II)}**

Acta Cryst. (2008). E64, m1435 (doi.org/10.1107/S1600536808033151)



The molecular coordination sphere of $[\text{Cu}(\text{CF}_3\text{SO}_3)_2(\text{C}_{16}\text{H}_{18}\text{N}_4)]$.

The molecular structure is composed of discrete neutral Cu^{II} units of $[\text{Cu}(\text{CF}_3\text{SO}_3)_2(\text{C}_{16}\text{H}_{18}\text{N}_4)]$, which have been derived from the flexidentate bis(pyridylimine) ligand, *N,N'*-bis[1-(pyridin-2-yl)ethylidene]ethane-1,2-diamine, in which the two pyridylimine binding units are linked by an ethylene spacer. The ligand acts as a tetradentate chelate in the equatorial plane and the weakly bonded triflate ligands above and below this plane complete the monomeric CuN_4O_2 chromophore of tetragonally distorted pseudo-octahedral geometry.

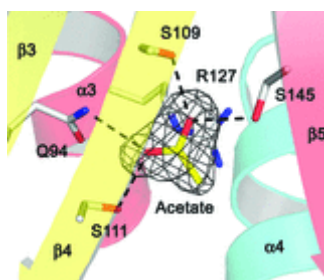
Simon J. Coles, Abdurrahman Sengul, Ozgur Kurt and Safinaz Altin

IUCR JOURNALS NEWS

Rv0802c from *Mycobacterium tuberculosis*: the first structure of a succinyltransferase with the GNAT fold

Rv0802c from *Mycobacterium tuberculosis*: the first structure of a succinyltransferase with the GNAT fold

Acta Cryst. (2008). F64, 978-985 (doi.org/10.1107/S1744309108031679)



Electron density ($F_o - F_c$ OMIT map at 4σ) for a bound acetate ion discovered serendipitously within the active site of 'unliganded' Rv0802c.

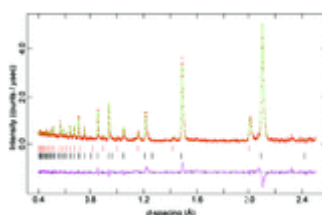
GCN5-related *N*-acetyltransferases (GNATs) typically transfer an acetyl group from AcCoA to a diverse set of amine-containing substrates. The structure of Rv0802c, a hypothetical GNAT from *Mycobacterium tuberculosis*, was determined and found to contain a multicoordinated acetate ion. The location of the acetate ion suggested an alternative acyl donor for Rv0802c, which was borne out by the structure determination of Rv0802c with bound succinylCoA. Structural analysis of Rv0802c was therefore crucial in revealing that a subset of GNAT family members can utilize succinylCoA as a cofactor.

M.W. Vetting, J.C. Errey and J.S. Blanchard

Thermoelastic properties of magnesiowüstite, $(\text{Mg}_{1-x}\text{Fe}_x)\text{O}$: determination of the Anderson-Grüneisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures

Thermoelastic properties of magnesiowüstite, $(\text{Mg}_{1-x}\text{Fe}_x)\text{O}$: determination of the Anderson-Grüneisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures

J. Appl. Cryst. (2008). 41, 886-896 (doi.org/10.1107/S0909049508029439)



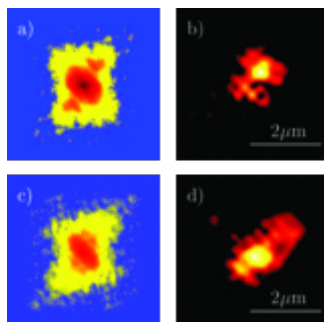
Rietveld refinement of a mixture of Fe (used to determine the pressure) and $\text{Mg}_{0.8}\text{Fe}_{0.2}\text{O}$ at 4.9 GPa and 390 K.

Seismic tomography and geodynamical modelling are major techniques for studying the Earth's lower mantle. Both methods require knowledge of how the elastic properties of mantle constituents, such as magnesiowüstite $[(\text{Mg},\text{Fe})\text{O}]$, vary with pressure, temperature and composition. The Anderson-Grüneisen parameter gives a measure of the rate of change of the bulk modulus with temperature, and the rate of change of the thermal expansion coefficient with pressure. We have used lattice parameter measurements by time-of-flight neutron powder diffraction at simultaneous high pressure and high temperature to determine this quantity.

I. G. Wood, L. Voadlo, D. P. Dobson, G. D. Price, A. D. Fortes, F. J. Cooper, J. W. Neale, A. M. Walker, W. G. Marshall, M. G. Tucker, D. J. Francis, H. J. Stone and C. A. McCammon

Coherent X-ray diffractive imaging of protein crystals

J. Synchrotron Rad. (2008). 15, 576-583 (doi.org/10.1107/S0909049508029439)



The new synchrotron radiation technique of coherent X-ray diffractive imaging using diffraction at a Bragg peak has been applied to the study of micrometer-sized protein crystals. Under coherent conditions, fringes appear on the Bragg peak, which are related to the crystal shape. In the highlighted work, the two-dimensional shape of the crystal was recovered from the diffracted intensity alone, using a real-space 'support' constraint. While radiation damage was a key limitation, this demonstration paves the way to the study of nanocrystals at free-electron laser sources, such as the Linac Coherent Light Source in 2009.

S. Boutet and I. K. Robinson

MEETING REPORT

XXI Congress and General Assembly IUCr2008



Osaka, Japan, August 23-31 www.iucr2008.jp/

continued from Volume 16, No. 3

Keynote Lectures

***Ab initio* powder diffraction studies of organometallics and coordination polymers (KN02)**



Angelo Sironi (U. of Milan, Italy) described the use of X-ray powder data to study organometallic compounds and coordination complexes. Patterson maps afford substantial information but the key to successful structure solutions generally comes from manipulating structural models within the crystal lattice. In recent years real-space methods have been developed, in which molecules or fragments are rotated and moved within the unit cell, until the simulated powder diagram is similar to the experimental one. If the coordination geometry of a metal ion is not known in advance, the metal atom and the organic ligands are treated as independent fragments. For the real-space procedure, as well as for the Rietveld refinement, Sironi applies the maximum-entropy method to highlight the presence of guest molecules using a self-developed link between the programs TOPAS and PRIMA.

Martin Schmidt

Focused structural genomics (KN34)



Andrzej Joachimiak, (USA), gave an overview of the Protein Structure Initiative (PSI) and structural genomics effort funded by the NIH Inst. of General Medical Sciences, and of the Midwest Center for Structural Genomics (MCSG). He discussed the goals of the current second stage of PSI efforts and the philosophy behind the target selection process. He pointed out that PSI researchers are now the major contributors of novel structures to the PDB. Joachimiak also described several protocols used at MCSG trying to improve the success rate of the overall structural determination process, including construct optimization, ortholog scanning, reductive methylation of lysine side chains, in situ proteolysis, and co-expression. He finished with examples from several focused genomics projects at the MCSG, including heat shock proteins, the TetR family of transcription factors, the Isd heme iron transporters, sortase inhibitors, and the identification of a novel virulence factor from the human pathogen *Pseudomonas aeruginosa*.

Liang Tong

Microsymposia

Automation of data acquisition (MS10)

Strategies for using a high-resolution, high-throughput powder diffraction beamline at the Advanced Photon Source (APS) providing mail-in operations were described by Brian Toby (USA). He outlined the requirements for sample tracking, data collection with a robotic sample exchanger, an automated data reduction and distribution system, the advantages of standardization and automation, how to achieve high resolution by optimizing performance of beamline optics and how to accomplish all of this with limited staffing. Lee Daniels (USA) outlined a completely automated single crystal processing system with optical crystal centering, X-ray screening, symmetry determination and detailed collection strategies, with an empirically tuned scoring system. He also pointed out that although we have access to hands-off crystallography, we still have a responsibility to provide hands-on training to the next generation of crystallographers. Joerg Kaercher (USA), resisted the temptation to mention commercial products while presenting the logic behind a completely automated single crystal pipeline, from sample quality checking and cell determination to report writing. The user could supply a crystal, propose a formula, distinguish sample decomposition from a wandering crystal, grab a coffee, and then publish. Highlighting remote access drug discovery Stephen Burley (USA) described a fully automated process including loop visualization/centering, crystal screening and data collection, crystal quality scoring and data processing/reduction performed at SGX-CAT (APS). What was once a data collection issue has become an exercise in data management? We were shown how refreshing a liquid nitrogen shower could be and how real-time input from an evolving sample database can enhance the automation process.

Michele Cianci (Germany) gave us the beamline scientist's perspective on the extensive testing and validation required to program decision-making algorithms for sulfur phasing protein crystallography. How does energy choice affect the dose, coverage, and phasing of various types of crystals? How to capitalize on redundancy of data collection, minimize radiation damage, and optimize wavelength, resolution, and absorbed dose to obtain the best data for sulfur phasing was presented.

We came away with the feeling that automatic data acquisition could be trusted to provide rapid analyses without compromising reliability or quality of the results.

James F. Britten and Jun Wang

Solid-state transformations of molecular solids (MS17)

This microsymposium covered photochemistry and 'dynamic' phenomena in molecular crystals including vapor induced transformation of platinum complexes (M. Kato, Japan), and mechanochemical solvent-free synthesis of metal-organic frameworks (S.L. James, UK).

In an opening address M. Kaftory (Israel, co-chair) summarized the recent history of solid-state photochemistry and observed that growth in the field may be traced to the work of Gerhardt Schmidt at the Weizmann Inst. of Science. The number of solid-state photochemistry publications grew rapidly in the 1990s due in great part to the contributions of John Scheffer who demonstrated asymmetric photochemical synthesis in the solid state using chiral salts and the late Fumio Toda who demonstrated solid-state photochemical synthesis using inclusion compounds. Kaftory paid tribute to Toda's work in organic solid-state chemistry and his major contributions to the field. Using time-resolved pink-Laue photography for direct observation of solid-state photo-isomerization and photo-reaction was discussed by P. Coppens (USA). Organic compounds that are difficult to synthesize can be formed easily by crystalline-state photoreaction. The formation of 'ladderane' compounds was demonstrated by L. R. MacGillivray (USA). New frameworks of traditional photochromism and thermochromism were presented by J. Harada (Japan). The combination of *in situ* structure analysis and spectroscopic studies of

salicylideneaniline crystals offered increased insight into chromic phenomena in crystals. The symposium was organized by members of the IUCr Commission of Structural Chemistry.

Hidehiro Uekusa

Time-resolved and coherent X-ray scattering (MS20)

This microsymposium covered applications of a wide range of synchrotron-based techniques to determine dynamical properties of non-crystalline systems, ranging from biological macromolecules to nanomaterials.

Satoshi Takahashi (Japan) highlighted their time-resolved SAXS studies of protein folding in the microsecond time domain by using a continuous-flow mixing device. They found a scaling relationship between radius of gyration and chain length in the early intermediates of various globular proteins, suggesting a chain-length dependency of coil-globule transition. Since SAXS provides an ensemble average a new technique was developed to record fluorescence resonance energy transfer (FRET) kinetics from single molecules. Interestingly, conformational dynamics within the unfolded state of iso-1-cytochrome c were relatively slower than the rates of the initial collapse probed with SAXS. Further comparison between the results from SAXS and single molecule FRET at even higher time resolution will usher in new insights on protein and RNA folding mechanisms. Stephan V. Roth (Germany) presented time-resolved grazing incidence X-ray absorption spectroscopy studies with micron-sized beams on growth kinetics during *in situ* sputter deposition of gold on organic polymer films.

Yuya Shinohara (Japan) focused on the reinforcement mechanism of carbon black/silica-filled rubber. The deformation of the silica-filled rubber was followed using time-resolved ultra SAXS in a pinhole SAXS instrument with a sample to detector distance of 160 meters at SPring-8. The structure factors of the fillers were extracted by dividing the observed 2D ultra soft X-ray absorption spectroscopy pattern by a simulated form factor of the spherical silica particle. To understand the dynamics in the rubber composites X-ray photon correlation spectroscopy (XPCS) was also used. Spatial arrangement of the fillers, visualized by Reverse Monte Carlo simulation of the resulting structure factors and the dynamics near glass transition temperature provided a relationship between the structure and mechanical property of the filled rubber.

Robert L. Leheny (USA) described the fundamentals of the XPCS technique using coherent X-rays to study the dynamics of soft glassy materials and gels. Auto-correlation functions of the disordered soft solids near their glass transition temperature could only be described by a compressed exponential decay and the derived characteristic relaxation times were found to be inversely proportional to the scattering vector (Q), rather than their square (Q^2) expected for simple diffusion. Many systems exhibited such a super-diffusive behavior near their glass transition and XPCS offers a unique window to investigate interesting physics in a wide range of nanostructured hybrid materials.

Qun Shen (USA) gave an overview of coherent X-ray diffraction imaging at APS. Development of a crystal guard aperture to eliminate undesirable parasitic-scattering background was the key to achieving higher signal-to-noise ratios of diffraction images. A comparison between transmission X-ray imaging and coherent diffraction imaging was demonstrated using an AgAu alloy in which dealloying was carried out through chemical etching.

P. Thiyagarajan and Shuji Akiyama

Photo-excited state crystallography (MS24)

A symposium on recent advances in time-resolved and steady-state photo-crystallography began with a report by S. Adachi (Japan) on the dynamics of shock-induced lattice deformation of single crystals of CdS, probed by time-resolved Laue diffraction at the Photon Factory (KEK, Tsukuba, Japan). From time-

resolved X-ray absorption fine structure, Adachi explained the structural reorganization attributed to the low spin to high spin conversion of the spin-crossover complex $[\text{Fe}^{\text{II}}(\text{phen})_3]^{2+}$. The [2+2] photo-dimerization process of α -styrylpyrylium proceeding in a picosecond timescale as a single-crystal-to-single-crystal transformation was described by J. Hallmann, (Germany). Using X-ray absorption spectroscopy with picosecond resolution, M. Chergui (Switzerland) followed the structural reorganization associated with the singlet to quintet photo-conversion of the spin-crossover complex $[\text{Fe}^{\text{II}}(\text{bpy})_3]^{2+}$, namely a $\sim 0.2\text{\AA}$ elongation of the Fe-N bonds. The contributions by P. Raithby (UK) and A. Phillips (UK) illuminated the crystal structures of metastable linkage isomers of Ni and Ru coordination complexes. In the case of $\text{Ru}(\text{SO}_2)(\text{H}_2\text{O})(\text{NH}_3)_4$, the metastable state consists of a Ru-O-S-O coordination mode. Rational strategies to reach high photo-conversion in the solid state were proposed and illustrated, such as the use of bulky side ligands.

Sébastien Pillet

Structure solution and refinement from powders (MS53)

Since the advent of the Rietveld method in the 1960s, progress in powder diffraction has accelerated with the development of pattern decomposition methods, direct-space methods (1990s), improved software for data analysis, routine applications to structural studies and continued development of algorithms and instrumentation. Masaki Takata (Japan) discussed electrostatic potential and electric field imaging techniques, emphasizing the usefulness of the electron density distribution derived by using the maximum entropy method. Maria Christina Burla (Italy) showed examples of the application of MAD techniques to synchrotron radiation powder diffraction data. Chick Wilson (Scotland), discussed ways of determining hydrogen positions with neutron powder diffraction. Vladimir Chernyshev (Russia) discussed DFT optimization in the analysis of crystal structures with a large number of variables. Kenneth Shankland (UK) discussed the analysis of solid solutions and the carbamazepine crystal structure landscape.

Hideo Toraya and Peter Stephens

Membrane protein structures (MS64)

While structure determination of membrane proteins remains challenging, continued advances in the techniques of sample preparation and crystallization are moving the field forward and success with difficult targets, including those of eukaryotic origin are being reported.

The structure of the plant photosystem I supercomplex, was presented by Alexey Amunts (Israel). Based on near-atomic models of more than 3,000 residues (168 chlorophyll molecules, 2 phylloquinones, 3 FeS clusters, and 5 carotenoids), Amunts outlined a proposed pathway of electron transport and discussed the molecular evolution of the complex based on structural comparisons with a similar complex in cyanobacteria. Bjørn P. Pedersen (Denmark), described the structure of a plant P-type ATPase plasma membrane proton pump having a characteristic cavity near charged or polar residues that are important for the transport function of the protein, and outlined a plausible proton-pumping mechanism that would open the cavity toward the exit and reposition the charged/polar residues. Both speakers offered tips on protein preparation and crystallization and ways to improve crystal quality, expedite data collection, and generate phases.

Di Xia (USA), determined the structure of the cytochrome bc_1 complex, a respiratory chain component, from a photosynthetic purple bacterium *via* the utilization of a mutant and inhibitors for protein stabilization, and a search for suitable sample preparation conditions (e.g. detergents) based on the properties of the target monitored by Blue Native-PAGE. Kenji Inaba (Japan), presented the crystal structure of a protein complex that is part of a disulfide-bond introduction system in the *E. coli* periplasmic space, captured by the use of a mutant that was elegantly designed based on previous

biochemical data. Inaba also examined a structural role for the horizontal α -helix found in a membrane protein using a series of chemical modification experiments, and revealed its significance for intermolecular disulfide formation.

A dynamic look at a membrane protein in the course of its function was demonstrated by Satoshi Murakami (Japan) who presented a new crystal structure for the bacterial multidrug transporter, AcrB, in which each protomer in the trimer has a different conformation. He suggested that the protomer structures represent the three phases of the drug transport cycle and proposed that they 'functionally rotate' in order through the various states. In the past, only single-state structures have been available for most membrane proteins in the Protein Data Bank owing to the difficulty of structural analysis. The accumulation of structural information under multiple physiological states, as presented by Murakami, may provide deeper insights into the functional mechanisms of membrane proteins.

Atsuko Yamashita

Multiferroic materials (MS74)

The field of the magnetoelectric coupling of multiferroic materials is reaping the benefits of experimental and theoretical advances. Yukio Noda (Japan) showed phase transitions involving simultaneously magnetic and dielectric ordering in multiferroic YMn_2O_5 and discussed the mechanism of introduced ferroelectricity, using neutron and X-ray scattering and electrical measurements. Michel Kenzelmann (Switzerland) discussed the use of phenomenological Landau type analysis to study ferroelectricity in spiral magnets (TbMnO_3 and $\text{Ni}_3\text{V}_2\text{O}_8$). Dimitri Argyriou (Germany) discussed the magnetoelectric phase diagram of $(\text{NdY})\text{MnO}_3$ with the fine tuning of the Mn-O-Mn bond angle, and magnetoelectrically coupled low-energy excitation in TbMnO_3 . Francoise Damay (France) described the frustrated antiferromagnet delafossite CuCrO_2 which had been recently found to be a magnetically driven ferroelectric and John Claridge (UK) discussed the design of multifunctional materials that can be made under ambient conditions.

Tsuyoshi Kimura, Loreynne Pinsard-Gaudart

Structural proteomics (MS85)

During the last 10 years, world-wide structural genomics efforts have resulted in the development of novel high-throughput technologies (e.g. nano-crystallization, robotics for crystal screening at synchrotrons), tools (salvage pathways, novel cloning strategies) and reagents (proteins and expression plasmids that have changed the field of structural biology). Those developed by the NIH Protein Structure Initiative, PSI, are now available to the entire community: www.hip.harvard.edu/PSIMR/index.htm). The focus of many structural genomics efforts is shifting towards structural proteomics, where these high-throughput technologies and methods are being applied to specific, biological problems.

Johan Weigelt, (Sweden, 650 protein structures in the PDB), described structural investigations of key regulators of apoptosis, and enzymes that covalently modify other proteins through poly(ADP-ribosylation) and play roles in DNA repair. One structure (tankyrase 1, TNKS1), is a potential drug target involved in telomere homeostasis. Surprisingly, one loop in TNKS1 was found to bind Zn. Zn-binding appears to play a role in stabilizing the protein fold and may be important for mediating protein:protein or protein:DNA interactions.

Ian Wilson (USA) highlighted progress at the Joint Center for Structural Genomics (JCSG), where a major goal is a full understanding of the biochemistry of a single organism, *T. maritima*. More than 315 unique *T. maritima* structures have been determined, (170 by JCSG) making *T.m.* the genome with the highest structural coverage (16%). These structures are beginning to provide structural coverage of all metabolic pathways. The JCSG now tracks 520 independent parameters per experiment, recorded at 32 different

stages of sample production, providing a wealth of experimental data. These data have been analyzed by the JCSG and used to develop freely available programs like XtalPred (ffas.burnham.org/XtalPred-cgi/xtal.pl), which predicts the likelihood that a protein will crystallize, and identifies the homologs that are most likely to crystallize.

Rebecca Page (USA) described a focused structural proteomics effort which combines NMR spectroscopy and X-ray crystallography to elucidate the molecular basis of phosphatase regulation. Their most exciting structure thus far was of the PP1:spinophilin complex. As shown using NMR spectroscopy the PP1-binding domain of spinophilin is completely unstructured in the unbound state. However, when bound to PP1, where it wraps around the surface of the phosphatase, it not only binds in an extended conformation but also forms new secondary structural elements that result in an extension of the central β -sheet of PP1. This is the first time that a PP1-regulatory protein has been demonstrated to bind PP1 in a surface pocket previously thought to be used exclusively by PP1 substrates.

Tuberculosis (TB) remains one of the most wide-spread and lethal diseases. Manfred Weiss (Germany) described the use of structural proteomics to understand the biology and life cycle of the pathogenic bacterium, *M. tuberculosis*. TB is a unique organism that contains all of the protein machinery required to live in any environment. Thus any one of its ~4000 proteins has the potential to be a target for novel drugs. Manfred described their structure of Rv2827c, an *M. tuberculosis* protein that is upregulated under survival conditions in macrophages. They found that Rv2827c is a DNA binding protein and a suitable target for the TB-based drug discovery programs. He also reported that the structure of 6 of the 9 proteins required for lysine metabolism are known. The active sites of these and the 40 other *M. tuberculosis* proteins determined by the XMTB Structural Proteomics Consortium EMBL group, provide a broad platform for international structure-based drug discovery programs.

Shigeyuki Yokoyama (Japan), described advances in elucidating the structural basis of protein synthesis via a comprehensive study of the structures of proteins and RNAs as diverse as tRNAs, aminoacyl-tRNA synthetases, translation factors and ribosomal subunits. The work spanned crystallography and electron microscopy and emphasized how these complementary techniques can be used to gain fundamental mechanistic insights into biological problems. Using both techniques, Shigeyuki was able to show that the conformations of a number of ribosomal binding proteins (determined using X-ray crystallography) change upon interacting with the ribosome (determined using electron microscopy) as well as how these changes can be modeled using both the crystal structures and the cryo-EM maps. He also described the recently determined crystal structure of ArgRS (arginyl-tRNA synthetase) that provides insights into how the cognate tRNA of this synthetase accelerate the ATP-Pi exchange reaction.

Rebecca Page

Programming for CIF and related file structures (MS96)

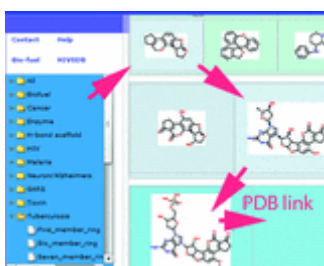
This session included presentations describing the new flavour of CIF that is based on the dictionary language and some recent CIF applications. Nick Spadaccini (Australia) outlined the new features of DDLm, while James Hester (Australia) showed how the algorithms encoded in the DDLm CIF dictionaries could be used to generate the values of missing CIF items at run time. The importance of the relational structure of CIF for archiving was emphasized by Herbert Bernstein (USA) who showed that, while a relational file structure could readily be transformed to other file types, the reverse transformation was much more difficult. Mois Aroyo (Spain) gave an example of a CIF-based archive, the Bilbao Crystallographic Server, which stores information on space groups and space group relations and Brian McMahon (UK) described pubCIF, an editor for generating CIFs for submission to *Acta Crystallographica*. He showed how pubCIF can insert a short Jmol script into the CIF, thus allowing a reader to use pubCIF to retrieve the author's interactive view of the structure directly from the CIF.

I. David Brown

Knowledge-based applications in structural chemistry (MS98)

The session spanned a wide range of topics linked by the common theme of structural databases as sources of knowledge.

Ramaswamy Subramanian (USA) described analysis of the quality of structures in the Protein Data Bank (PDB) as a function of parameters, such as date of deposition, resolution and number of atoms in the structure. Individual structures could then be assessed in terms of the expected quality of similar structures in the PDB. A number of trends could be seen, including the observation that high-impact journals tend to feature poorer quality structures! Jacqueline Cole (UK) described the typical characteristics of organic nonlinear optical materials, namely the presence of an electron donor/acceptor pair, a π -conjugated system and bond-length alternation. Structures in the Cambridge Structural Database (CSD) could be mined for these features using a 'Molecular Lego' approach. The top hits correlated well with semi-empirical and DFT calculations of the hyperpolarisability and with known nonlinear optical materials.



Chem-BLAST facilitates the searching of ligands in PDB and HIVSDB using a Chemical Structural Ontology presented in multiple layers as images of popular scaffolds <http://xpdb.nist.gov/pdb/chemblast.html>.

(Courtesy of T. N. Bhat)

A different application of the CSD was presented by Susanne Huth (UK) who surveyed 24 members of the pharmaceutically-important para-acetanilides family. The Southampton programme XPac was used to investigate and compare 1D, 2D and 3D hydrogen bonding patterns allowing the 24 structures to be grouped into a hierarchy of crystal packing forms. Lattice energies were also calculated but showed poor correlation with structural properties. Deuteration of proteins is known to lead to functional changes (D_2O is toxic!) but, with two known exceptions, it is assumed to lead to no significant structural changes. With a lack of suitable comparisons in the protein world, Stuart Fisher (UK) turned to the CSD and compared deuterated compounds with their equivalent hydrogenated compounds. The maximum shift in position found was $0.3\text{\AA}$ which is not significant at the usual resolution of protein structures. Talapady Bhat (USA), described the HIV structural database which contains structural and biochemical data on inhibitors, drug leads and clinical drugs for AIDS. He pointed out that AIDS research presents one of the best success stories of structure-based drug design. He discussed the problem of searching for small molecule ligands when you are not sure what you want, and presented the tool Chem-BLAST which allows a tree-based graphical search for structural fragments.

Martyn Winn

New algorithms for understanding magnetic structures (MS61)

This microsymposium provided an overview of the computational means by which magnetic structures may be deduced from neutron diffraction data. An important step in determining magnetic structures involves symmetry analysis and the symposium began with an introduction to Representation Theory and Analysis by Andrew Wills (UK) author of the *SARAh* program. Andrew's talk was complemented by a presentation of *SARAh* at the Software Fayre, organized by Lachlan Cranswick. Juan Rodríguez-Carvajal (France), the author of *FullProf*, focused on the use of Simulated Annealing to determine magnetic structures and this talk was also complemented by a presentation at the Software Fayre. A more theoretical approach was provided by Daniel Litvin (USA) who discussed the use of magnetic space

groups and provided a useful link to his recent Electronic Book tabulation of all magnetic space groups, effectively an International Tables for Magnetic Crystallography (www.bk.psu.edu/faculty/Litvin/V1.2_Magnetic_Space_Groups_Book.pdf). Andrew Goodwin (UK) described Reverse Monte Carlo methods, with reference to the program RMCProfile. A key point here is that local structure information which may be inaccessible by traditional Rietveld refinement techniques may be modeled using RMC methods. The symposium finished with an experimental talk by Chih-Hao Lee (Taiwan) in which he described the Magnetic Circular Dichroism method, illustrated with reference to recent work on FePt ultra-thin films.

The microsymposium was chaired by Seán Cadogan (Canada) and Max Avdeev (Australia).

Seán Cadogan

Future of Female Crystallographers

Activities to increase the number of women scientists in each country



Speakers and Chair. In front: I. Margiolaki, J. A. K. Howard, L. N. Johnson, J. P. Glusker; in back: K. Kurihara, Y. Ohashi, A. Takenaka, T. Kiyotani.

The 2008 IUCr Congress presented an excellent opportunity to talk about problems facing crystallographers. A special evening session dealing with this issue was titled 'Future of Female Crystallographers'. The session was organized by the Crystallography Society of Japan (CrSJ), and the organizers were Tamiko Kiyotani (Chair), Midori Kamimura, Satoshi Sasaki, Akiko Sekine and Nobutada Tanaka. All participants, ladies, gentlemen, students and senior scientists, were welcomed, and there were 89 participants from 23 countries.

The session opened with introductory comments from Akio Takenaka (CrSJ President) and Yuji Ohashi (IUCr President). The audience then heard from 5 invited speakers who represented female crystallographers from various parts of the world: Kazue Kurihara (Japan), Jenny P. Glusker (USA), Judith A. K. Howard (UK), Louise N. Johnson (UK) and Irene Margiolaki (France).

The lectures were followed by a mixer with snacks and drinks during which all participants engaged in active and lively discussions on the theme of the session. For young scientists, it was a good chance to interact with more experienced scientists in the field. The entire session was very lively, serious and significant.

If crystallography is to continue to evolve and grow it is very important to continue to consider and discuss problems that surround young scientists entering the field. The organizers sincerely hope that all participants will continue to promote such discussions and interactions and that similar sessions will be organized at future IUCr Congresses.

Tamiko Kiyotani



Left: IUCr Journal Editors and Coeditors at the Journals Commission Satellite Meeting. (Photo courtesy of Karl Törnroos) Right: Past IUCr President, Theo Hahn, flanked by the paparazzi. (Photo Courtesy of W. L. Duax)



Left: The IUCr Executive Committee meeting in session in Osaka. Left-hand side, front to back: P. Colman, C. Lecomte, G. Heger, G. R. Desiraju, C. J. Gilmore, M. Cooper, W. L. Duax, G. Kostorz; Right-hand side, front to back: I. Torriani, D. Viterbo, P. Strickland, S. Liden, Y. Ohashi, M. Dacombe, Jane Robinson. Right: Staff members Sae Ishikawa and Hiroshi Kikuchi. (Photo courtesy of Ross Doyle)



Left: Participants at the Workshop on New Routes to Crystallographic Data Publication. Right: Brian McMahon (IUCr) speaking at the workshop. (Photos courtesy of Simon Coles)

MEETING REPORT

2008 Crystallographic Computing School

Kyoto, Japan, August 18-23, 2008

Images from the crystallographic computing school. (Photos courtesy of Yu Jian.)

The traditional IUCr crystallographic computing school was organised and run by the IUCr computing commission in Kyoto and held just prior to the IUCr congress in Osaka. The location was the Kansai Seminar House nicely located in the hills around Kyoto and close to one of the many temple complexes for which Kyoto is well known. The school brought together a group of about 50 crystallographers interested in the development of crystallographic software. The program consisted of lectures by senior crystallographers, tutorials and presentations by young participants of their own work in crystallographic software. The leading theme of the school was the transfer of the knowledge of the older, soon to retire generation of developers, to the next generation of developers. The program of the school was designed to be attractive for both small-molecule and macromolecule crystallographers. The presentations of the meeting have been collected in issue #9 of the newsletter of the computing commission and can be downloaded from www.iucr.org/resources/commissions/crystallographic-computing/newsletters/9.

Photographs made during the school by Jian Yu can be found on the WEB-site of the computing commission. Thanks are due to the local organiser, Min Yao, who did an excellent job in making things work in an environment foreign to us and the various sponsors that allowed us to keep the participant fees as low as possible.

Ton Spek, Chairman

MEETING REPORT

BioCrys2008

Oeiras, Portugal, October 2008

Participants at the BioCrys2008 course in Oeiras, Portugal.

The fourth BioCrys course on 'Fundamentals of modern methods in biocrystallography' was organized by Maria Arménia Carrondo (ITQB Oeiras, Portugal) and Thomas Schneider (EMBL Hamburg, Germany). It brought together 35 students from 15 countries and 19 tutors from 8 countries. The aim of the course was to teach the fundamental concepts of macromolecular crystallography to scientists in the early stage of their crystallographic career. Lectures and tutorials covered topics from the cooling of crystals to the validation of the final structural model. A cluster of 18 Linux computers was set up by Pedro Matias (ITQB, Portugal).



Elspeth Garman teaching the practical side of crystal cooling and data collection.

Ed Hough (U. Tromsø, Norway) laid out the basics of crystallography in real and reciprocal space.

Christoph Hermes (EMBL Hamburg, Germany) gave an overview about the principles of X-ray sources and X-ray detectors and Elspeth Garman (Oxford U., UK) covered the practical side of crystal cooling and data collection. Kevin Cowtan (York U., UK) guided the students through the world of structure factors and how they relate to electron densities in his web-based tutorial (www.yorvic.york.ac.uk/~cowtan/sfapplet/sfintro.html). A tour of crystallographic resources on the world wide web was presented by Isabel Bento and Colin McVey (both ITQB, Portugal). The first two evenings started with ice-breaker sessions during which all participants gave 2-min presentations of their current work.

Strategic questions of data collection and both theoretical and practical aspects of data processing were addressed by Zbyszek Dauter (Argonne Nat. Lab., USA) and Andrew Leslie (MRC Cambridge, UK) and included practicals on integration and scaling of diffraction data. Gordon Leonard (ESRF Grenoble, France) gave an introduction to the use of anomalous scattering in macromolecular crystallography. The substructure solution process and MAD-phasing were covered by Thomas Schneider. Kevin Cowtan discussed the principles of the different density modification techniques used for phase improvement and Zbyszek Dauter explained SAD-phasing. Molecular Replacement was introduced by Gabor Bunkoczi (Cambridge U, UK). Carlos Frazão (ITQB,) described how the particular problems that one encounters with twinned crystals can be tackled.

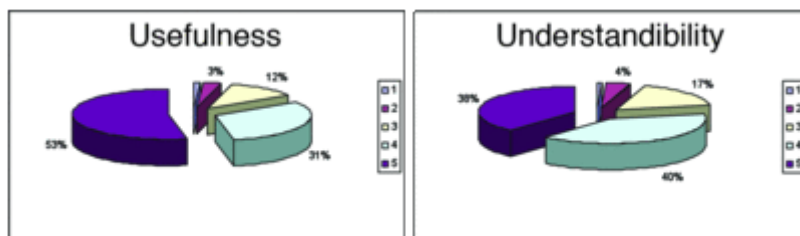
The MIR-method was discussed and later practiced in a tutorial by Clemens Vornrhein (GlobalPhasing Cambridge, UK), Kevin Cowtan covered the use of maximum likelihood in crystallography. Various aspects of symmetry were covered in a two hour tutorial on 'How to read (and understand...) the

International Tables' given by Zbyszek Dauter. Thomas Schneider lectured on refinement and the importance of taking into account model precision in the interpretation of structural data.

Automated model building and refinement were discussed both from a methodological and practical point of view by Anastassis Perrakis (NKI, The Netherlands). Gabor Bunkoczi demonstrated the use of PHASER for molecular replacement. Bernhard Lohkamp (Glasgow U., UK) taught the principles and practicalities of manual model building. The discussion of model building was complemented by an overview about the tools and concepts for assessing the correctness of a model by different validation criteria by Alekos Athanasiadis (ITQB). The course closed with a tutorial on model refinement and completion run by Isabel Bento and Daniele De Sanctis (ITQB).

Most days concluded with an evening lecture, about a current topic in structural biology and included lectures on HTP cloning and expression screening by (Nick Berrow, IRB, Spain), structure determination of 'Big guys' (Nuria Verdagauer, IRB), and a presentation on the preparation of proteins for crystallization by Colin McVey.

The City Council of Oeiras invited all participants to dinner in Algés, where they had a hands on introduction to regional folk dancing.



'Usefulness' and 'Understandability' were evaluated on a scale from 1 to 5 ('no use' to 'very useful' and 'more confused than before' to 'I saw the light'). The questionnaires were returned by 35 participants. The results are summarized here.

The course was supported by the MAX-INF2 network (www.ccp4.ac.uk/maxinf, [RICA-CT-2004-505977]), the SPINE2-Complexes Integrated project (www.spine2.eu/SPINE2, LSHG-CT-2006-031220), the Support Action TEACH-SG (www.teach-sg.eu/TeachSG, LSSG-CT-2007-037198) and Fundação para a Ciência e Tecnologia (www.alfa.fct.mctes.pt/facc). We are grateful to the informatics staff of ITQB and EMBL Hamburg and Mafalda Mateus for administrative assistance.

Maria Arménia Carrondo and Thomas R. Schneider

MEETING REPORT

Fifth Belgian Crystallography Symposium

Brussels, Belgium, October 2008



Speakers at the Fifth Belgian Crystallography Symposium BCS-5. From left to right: S. De Feyter, G. Chapuis, J. Helliwell, H. D'Hondt, P. Nockemann, J.-L. Ferrer.

More than 85 scientists took part in the Fifth Belgian Crystallography Symposium BCS-5, held under the auspices 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 interdisciplinary contacts between Belgian scientists who use diffraction and microscopy techniques for atomic scale studies in the apparently unrelated fields of condensed matter chemistry and physics, material 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: 'Cracking lobster shell protein structures' by John Helliwell (Manchester, UK), '2D crystal engineering: from patterns to function' by Steven De Feyter (Leuven, Belgium) and 'Crystallographic excursion in superspace' by Gervais Chapuis (Lausanne, Switzerland). A poster session and commercial exhibition was organized during lunchtime. For the afternoon session three oral presentations were selected from the submitted abstracts (J. L. Ferrer, Grenoble, France; H. D'Hondt, Antwerp, Belgium; P. Nockemann, Leuven). At the end of the meeting two poster prizes were awarded to S. Cabus and F. Robert. This BCS-5 meeting was sponsored by the Royal Academies of Sciences and Art of Belgium, and by the firms Bruker AXS, Oxford Diffraction, Isogen Life Science, Goffin Meyvis, FEI Europe and JEOL.

Luc Van Meervelt

NOTICE

The Crystallographic Society of Japan



www.crsj.jp/index-e.html

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Term: April 2008 to March 2010

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NOTICE

Available synchrotron membership shares for protein crystallography at Argonne



Procter and Gamble (P&G) is interested in selling its membership shares in the Southeast Regional Collaborative Access Team (SER CAT) at Sector 22, a pre-eminent protein crystallography facility located at the synchrotron source of Argonne.

The available membership shares offer a full range of capabilities at scheduled visits throughout the year with two days of contiguous experiment times per visit.

The facility consists of a consortium of 25 member institutions with dedicated capabilities to high-resolution macromolecule crystallography, rational drug design, protein engineering and site-directed mutagenesis. It has both ID and BM sources, and a reputation around the world for high productivity in publications and PDB depositions.

For interest regarding purchase/lease options of P&G's membership shares, please contact 513-627-2437, or Email: wireko.fc@pg.com