

both enzyme families, the shuttle disulfide determines the substrate specificity. Furthermore, both the Ero1 and Erv2 families can transfer electrons to a similar panel of electron acceptors. One striking difference between the two enzymes, however, is that Ero1 displays kinetic complexities not shared by Erv2. This difference will be discussed in light of the structures, a mechanistic model will be presented, and a possible physiological role for the complex behavior of Ero1 will be suggested.

Keywords: flavoenzymes, disulfides, enzyme mechanisms

KN15.26

Acta Cryst. (2005). A61, C4

Synthetic Crystallography

A. Guy Orpen, *School of Chemistry, University of Bristol, Bristol BS8 1TS, United Kingdom.* E-mail: guy.orpen@bris.ac.uk

The synthesis of new and designed crystal structures is part of a major strand of modern chemistry in which the focus has shifted from the analytical function of crystallography (the determination of crystal structures) to the synthetic. In synthetic crystallography, itself a branch of crystal engineering, a variety of means have been used in the attempt to plan and control the products and objectives of synthesis – the crystal structures.

Here strategies that might be adopted to achieve this synthetic goal are considered. In particular the utility of approaches based on supramolecular chemistry and molecular tectonics are examined. Progress is evaluated towards control of:

- The composition of the final synthetic product - the crystal structure*
- The supramolecular synthon formed.*
- The periodic motif(s) formed.*
- The entire crystal structure.*

Applications and properties of such "engineered" solids is of importance. One property of particular interest to chemists is reactivity – this at the heart of the history of crystal engineering and has received sustained attention from a relatively small number of groups, primarily in solid state organic and organometallic chemistry. The prospects for the application of supramolecular crystals in synthesis and the opportunity to exploit the unusual constraints they impose on molecular reactivity are considered.

Keywords: crystal engineering, supramolecular crystallography, inorganic solid-state chemistry

KN16.26

Acta Cryst. (2005). A61, C4

A Perspective on the Crystal Structures of High Pressure Elements and their Properties

John S. Tse, *Department of Physics and Engineering Physics University of Saskatchewan, Saskatoon, Canada S7N 5E2. Steacie Institute for Molecular Sciences National Research Council of Canada, Ottawa, Canada K1A 0R6.* E-mail: John.Tse@usask.ca

Recent advancements in instrumentations and improvements in structural refinement techniques have led to the characterization of many structures of solids at high pressures. Some of the structure types discovered is novel and not seen in solids under ambient conditions. Even for elemental solids, particularly at intermediate pressure regime, it was found that instead of adopting simple close-pack structures, open and complex structures, modulated structures or incommensurately modulated structures were often observed. These observations challenge the conventional concept of chemical bonding for solids and provide a fertile ground for the investigation of new physical phenomena in materials under high pressure. In this presentation, high pressure structures and transformations on specific elemental solids are illustrated and discussed. The purpose is to develop a conceptual framework for the description of the structures and the understanding of the nature of chemical bonding at high pressure. It is shown that the distinct electronic structure and structural features are related to other unusual properties such as superconductivity.

Keywords: high-pressure structures, electronic structure calculations, chemical bonding theory

KN17.27

Acta Cryst. (2005). A61, C4

Some New Insights in to the Mechanisms of Fullerene and Nanotube Formation

Harold Kroto, *Chemistry Department, Florida State University, FL, USA. Chemistry Department, University of Sussex, UK.* E-mail: kroto@sussex.ac.uk

In 1985 Buckminsterfullerene (the third allotropic form of carbon) was discovered during experiments designed to unravel the chemistry in red giant carbon stars. The molecule has now come down to Earth giving rise to the Fullerenes, a family of pure carbon cage molecules with fascinating properties which promise exciting new developments in 21st Century Materials Science and Technology. Fullerene molecules and their elongated nanotube (buckytube) cousins are now the subject of intense study as they promise to play major roles in almost every possible area of future technology from medicine and molecular electronics to civil engineering. However the mechanisms whereby various types of nanostructures assemble are still very poorly understood. Over the last decade or so, we have examined a wide range of methods for nanotube formation and from these studies some interesting new insights have been gained – especially with regard to metal catalysed nanostructure formation.

Keywords: fullerene, nanotube, C60

KN18.27

Acta Cryst. (2005). A61, C4

Protein Kinase Inhibition and Substrate Recognition

Louise N. Johnson, *Laboratory of Molecular Biophysics, Biochemistry Department, University of Oxford.* E-mail: louise.johnson@biop.ox.ac.uk

Protein kinases are key components of cell signalling pathways. Defects in these processes lead to diseases such as cancer, diabetes and arthritis and hence protein kinases have become targets for drug design and therapy. We recently reviewed progress in this field with reference to kinase inhibitors that are in clinical trials or in the clinic and for which structural information is available[1]. In this talk I shall review some of our work with reference to cell cycle protein kinases [2] and I shall expand the discussion to consider wider aspects of substrate recognition with reference to CDK2/cyclin A, CDK2/cyclin E[3], CDK7 [4] and polo-like kinase[5].

[1] Noble M.E., Endicott J.A., Johnson L.N., *Science*, 2004, **303**, 1800. [2] Davies T.G., Bentley J., et al., *Nature Structural Biology*, 2002, **9**, 745. [3] Honda R., Lowe E.D., Dubinina E., Skamnaki V., Cook A., Brown N.R., Johnson L.N., *EMBO J.*, 2005, **24**, 452. [4] Lolli G., Lowe E.D., Brown N.R., Johnson L.N., *Structure (Camb)*, 2004, **12**, 2067. [5] Cheng K.-Y., Lowe E.D., Sinclair J., Nigg E.A., Johnson, L.N., *EMBO J.*, 2003, **22**, 5757.

Keywords: protein kinases, inhibitors, cell cycle

KN19.27

Acta Cryst. (2005). A61, C4-C5

Crystallography in Inorganic Solid-State Chemistry

James A. Ibers, *Department of Chemistry, Northwestern University, Evanston, IL 60208-3113, U.S.A.* E-mail: ibers@chem.northwestern.edu

The pervasive importance of crystallography, particularly results obtained from single-crystal studies, in inorganic solid-state chemistry will be explored through a number of examples of metal chalcogenide systems. These examples will also illustrate the importance of other physical measurements in the characterization of such compounds. Among such examples, the AMM'Q₃ system (A=alkali metal; M=f-element; M' = d-element; Q=S, Se, or Te) will be used to emphasize the importance of concomitant optical and magnetic measurements and the compound RbVSe₂ will serve to illustrate the importance of theoretical calculations.

There are also pitfalls and difficulties in the applications of crystallography to solid-state systems. The determination of chemical composition through the refinement of site occupancies is one of the most highly abused areas. Some aspects of the refinement of site occupancies will be explored through the NaLiM'S₂ series and the Er₂

$x\text{Sm}_x\text{Se}_3$ system. Comparisons will be made with quantitative chemical analyses obtained through the use of inductively coupled plasma (ICP) analyses.

Finally, the compound $\text{Ba}_4\text{Fe}_2\text{I}_5\text{S}_4$ will be used to illustrate the structural challenges posed by the unexpected in solid-state syntheses.

Keywords: metal chalcogenides, chemical crystallography, physical properties structure relationships

KN20.27

Acta Cryst. (2005). A61, C5

The Importance of Structure in the Design of Lithium Battery Materials

Michael Thackeray, Argonne National Laboratory, Argonne, Illinois 60439, USA. E-mail: thackeray@cmt.anl.gov

Since 1990, rechargeable lithium batteries have made a huge impact in powering consumer electronic devices such as cell phones and laptop computers [1]. The need for new insertion electrode structures that will provide additional energy, power and a superior cycle life to satisfy the increasing demands for reliable and safe high-energy/high power batteries by the transportation, medical, space, and defense sectors will ensure that lithium battery research will continue for many more years to come. This presentation will review the progress that has been made over the past 15 years and it will highlight the critical role that structure plays in the design and operation of lithium battery electrodes. Recent advances that have been made in designing two-component, structurally-integrated materials to achieve performance objectives will be discussed [2, 3]. The presentation will be made in the context of the advantages and limitations of other battery systems.

[1] Tarascon J.M., Armand M., *Nature*, 2001, **414**, 359. [2] Kim J-S., Johnson C. S., Vaughney J. T., Thackeray M. M., Hackney S. A., Yoon W., Grey C. P., *Chem Mater.*, 2004, **16**, 1996. [3] Thackeray M. M., Johnson C. S., Vaughney J. T., Li N., Hackney S. A., *J. Mater. Chem.*, 2005, *in press*.

Keywords: lithium battery, insertion electrode, structure

KN21.28

Acta Cryst. (2005). A61, C5

Pore-Forming Toxins

Michael W. Parker, Biota Structural Biology Laboratory, St. Vincent's Institute of Medical Research, Melbourne, Victoria 3065, Australia. E-mail: mparker@svi.edu.au

Pore-forming protein toxins (PFTs) are one of Nature's most potent biological weapons. They are produced by a variety of living organisms, particularly bacteria, certain insects, poisonous reptiles and stinging marine invertebrates. As offensive weapons these toxins can aid digestion or degeneration of the host whilst as defensive weapons they can protect by killing invaders. Of the more than 300 protein toxins characterized to date, at least a third act by disrupting membranes. In order for these water-soluble proteins to insert into membranes they must undergo a series of conformational changes to expose or generate new hydrophobic surfaces that can penetrate the core of cell membranes.

We have determined the crystal structures of a number of microbial pore-forming toxins. Although the structures are quite different they reveal common features that have been implicated in the mechanism of membrane insertion into cells. Two of these toxins belong to the family of cholesterol-dependent cytolysins (CDCs). CDCs exhibit a number of unique features amongst pore-forming toxins including an absolute dependence on the presence of cholesterol-rich membranes for their activity and the formation of very large oligomeric transmembrane pores greater than 15 nm in diameter. The crystal structures of these toxins suggest how they recognise cholesterol and provide the basis, together with available cryoelectron microscopy data, for modelling their pores.

Keywords: toxins, channel proteins, membrane associated proteins

KN22.28

Acta Cryst. (2005). A61, C5

Pressure Induced Complexity in the Elements

Malcolm McMahon, School of Physics and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh EH9 3JZ, U.K. E-mail: mim@ph.ed.ac.uk

At ambient pressure, the metallic elements typically adopt high-symmetry crystal structures such as bcc, fcc and hcp. However, on compression, many of these simple structures undergo a series of structural transitions to phases characterised by considerable structural complexity, and it is only with recent advances in high-pressure single-crystal and powder-diffraction techniques that many of them have been determined. In the group 1, 2, and 15 elements, we have found a number of incommensurate "hotel" structures comprising interpenetrating host and guest structures [1]; transitions between these composite structures [2]; modulations of the host and guest structures; a transition to a composite structure with a "liquid" guest component [3]; and a number of surprisingly complex commensurate structures. And in the group 16 elements, we have found a number of incommensurately modulated structures that are stable over a remarkably wide range of pressures and temperatures [4]. I will review all the recent results on these "simple" metals, and discuss possible explanations for the existence of this complexity.

[1] McMahon M. I., Degtyareva O., Nelves R. J., *Phys. Rev. Lett.*, 2003, **85**, 4896. [2] Nelves R. J., Allan D. R., McMahon M. I., Belmonte S. A., *Phys. Rev. Lett.*, 1999, **83**, 4081. [3] McMahon M. I., Nelves R. J., *Phys. Rev. Lett.*, 2004, **93**, 055501. [4] Hejny C., McMahon M. I., *Phys. Rev. Lett.*, 2003, **91**, 215502.

Keywords: incommensurate phases, high pressure physics, metals

KN23.28

Acta Cryst. (2005). A61, C5

Electrostatic and Related Properties from Accurate Charge Density Analyses

Mark Spackman, Chemistry - M314, University of Western Australia, Crawley WA 6008, Australia. E-mail: mas@cyllene.uwa.edu.au

Properties of atoms and molecules in crystals are now commonly extracted from a combination of X-ray diffraction experiments and theoretical results from a variety of approaches. Modern quantitative charge density studies typically involve use of CCDs and/or synchrotrons, T below 120 K and frequently nearer 10 K, careful data reduction and correction for systematic effects, and detailed modelling of atomic motion. Multipole refinement yields topological properties of the electron density in almost all studies, while valuable electrostatic properties are seldom reported. Yet there is a wealth of such properties accessible from the X-ray experiment: electrostatic potential, electric field and field gradient, atomic charges, electric moments of molecules in the crystal, and even intermolecular interaction energies.

If we accept that "theory is a good thing but a good experiment is forever" [1], we must ask: Are we maximizing the information that can be obtained from charge density data sets? If not, why not, and how might this be redressed? This presentation will seek answers to these questions from a discussion including results from a selection of recent studies. Limitations of some of the common approaches will be highlighted, and some solutions will be proposed, along with comments on related properties that might be explored.

[1] Kapitzka P.L., *Experiment, Theory, Practice*, (D. Reidel, Boston), 1980, 160.

Keywords: charge density studies, electron density studies, electrostatic properties

KN24.28

Acta Cryst. (2005). A61, C5-C6

Structural and Functional Studies of Large Macromolecular Assemblies

Nenad Ban, Department of Molecular Biology and Biophysics ETH Honggerberg, CH-8093 Zurich, Switzerland. E-mail: ban@mol.biol.ethz.ch

The main goal of the research in my laboratory is to study structure and function of large macromolecular assemblies involved in central cellular processes. Although most of our work focuses on