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

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Synthetic Crystallography

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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 :

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

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

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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

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

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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

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Protein Kinase Inhibition and Substrate Recognition

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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

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Crystallography in Inorganic Solid-State Chemistry

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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'Q_3 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 $RbVSe_2$ 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'S_2 series and the Er_2-