specificity and binding energies.

The availability of atomic resolution X-ray data allows refinement of anisotropic displacement parameters (ADPs) that complement the 3D coordinates. The information extracted from the ADPs gives insight into the mobility and the presence of ligand induced directional motion in the protein. Together with the change of contact distances and the occurrence of multiple conformers they reflect spatial rearrangement or steric strain. Thus, the analysis of the ADPs complements the time-averaged structural picture with dynamics, revealing subtleties of protein function which may not be attainable if a structure is analyzed only on the basis of the atomic coordinates.

A thorough analysis in terms of accessible conformational states deduced from the directional motion, may provide insight into the energetics of complex formation and the driving forces for allosteric mechanisms.

Examples for application of these analysis methods and their implication for protein structure interpretation will be given.

Keywords: intermolecular contacts, intramolecular contacts, protein structure

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Protein-Protein Interactions in the Cyanobacterial KaiABC Circadian Clock

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Circadian clocks are self-sustained biochemical oscillators. Their properties include temperature compensation, a time constant of approximately 24 h, and high precision. These properties are difficult to explain by known biochemical reactions. The ultimate explanation for the mechanism of these unusual oscillators will require characterizing the structures, functions, and interactions of their molecular components. We are analyzing the biological clock in the simplest cells that are known to exhibit circadian phenomena, the prokaryotic cyanobacteria, whose basic clock is composed of three essential genes, *kaiA*, *kaiB* and *kaiC* [1]. The structures of all three Kai proteins have recently been reported ([2], reviewed in [3]), along with phosphorylation sites in KaiC that are crucial for sustaining the oscillation [4]. Very recent research has demonstrated that the KaiABC clock keeps time in the absence of a transcriptional-translational oscillatory feedback loop [5] and that the circadian oscillation of KaiC phosphorylation can be reconstituted *in vitro* [6]. This means that the clock made up of recombinant KaiC, KaiA and KaiB proteins in the presence of ATP and Mg^{2+} ticks in an Eppendorf tube! The presentation will summarize the status of structural work on Kai proteins and efforts to begin to understand their complexes.

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Keywords: protein-complexes, protein-crystallography, protein-phosphorylation

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Unusual Ion Coordination in Membrane Channels and CH Hydrogen Bonds in Enzyme Catalysis

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Non covalent interaction play a critical role in ion transport by the membrane channel forming antibiotic gramicidin A and in the mechanism of catalysis in short chain oxidoreductase (SCOR) enzymes. Gramicidin A, a pentadecopeptide composed of alternating d and l residues, form a nanotube long enough to extend across a lipid bilayer and large enough to allow an unsolvated monovalent cation to move through the membrane. The inner surface of the nanotube is lined by π orbitals associated with peptide bonds and conjugated carbonyl groups. Ion coordination with these π orbitals are the driving force in ion transport. A pattern of strong C-H..O=C hydrogen bonds between carbon atoms on the nicotinamide ring of the NAD cofactor and the backbone carbonyl is of a Pro-Gly sequence in SCOR enzymes indicates that these interactions facilitate hydride transfer in the enzymes. Funded in part by NIH grant No. DK26546.

Keywords: cation-II interaction, C-H hydrogen bonds, natural nanotube

MS18 Powder Diffraction on Micro- and Mesoporous Materials

Chairpersons: Christian Baerlocher, Sergey Krivovichev

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Structure Determination of Zeolites: Making all the Pieces Fit

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In recent years new powder diffraction programs such as FOCUS [1] and EXPO [2] and simulated annealing techniques [3] have been developed to help solve zeolite structures, since these microporous materials are typically synthesized with crystal sizes too small for conventional single crystal structure determinations. Auxiliary techniques are usually employed to assist the researcher in solving a new framework structure. A correct unit cell and space group determination can be aided by electron diffraction, and the number of unique T-atoms and their connectivity can be determined by MQMAS and MQ-HETCOR NMR techniques. Gas absorption measurements indicate the size of the micropores and the dimensionality of its channels, while crystal density gives information about the total number of tetrahedral atoms in the unit cell.

A successful structure determination should not only ensure that the calculated diffraction pattern closely matches the experimental pattern, but also that *all the pieces fit,* i.e., all the characterization data support the proposed model. The above-mentioned and other techniques were used to elucidate the structures of zeolites ECR-34 and SUZ-4 and the aluminophosphates ECR-40 and EMM-3. The supporting characterization data were found to be essential for determining these new structures from powder diffraction data.

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Keywords: X-ray powder diffraction, zeolites, NMR spectroscopy

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Structural Characterisation and Properties of New Microporous Materials

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Zeolites are crystalline, hydrated aluminosilicates with open three-dimensional structures built of SiO_4 and AlO_4 *tetrahedra* linked to each other by sharing all the oxygens to form regular intracrystalline cavities and channels of molecular dimensions. These materials possess remarkable physical and chemical properties, such as selective adsorption, ion exchange and catalytic activity.

Mixed octahedral-pentahedral-tetrahedral (heteropolyhedra) microporous (OPT) framework silicates are zeolite-type materials synthesised and comprehensively studied since the early 1990s [1]. Examples include silicates of Ti and other metals, such as Zr, Nb, V and Sn and Cu. With the advent of the nanotechnology era, and the increasing interest in the use of molecular sieves for device applications, the constituent elements of OPT materials have been further extended to the lanthanide metals, exploring properties like photoluminescence [2].

OPT materials are often prepared in the form of microcrystalline powders (sometimes with considerable degree of disorder) and, thus,