

Microsymposia

means to manipulate micron sized objects in solution. A laser is focused by a high NA objective lens to produce an optical trap. Trapped crystals can be manipulated within the crystallization drop to both sort and mount them on standard crystal supports used in cryo macromolecular crystallography. The talk will demonstrate several successful examples of this new mounting technique and discuss the limitations like laser beam induced radiation damage.

Keywords: optical trapping, laser tweezers, microcrystals

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Serial crystallography using protein beams

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By spraying aligned molecules continuously across a synchrotron beam, we hope to develop a new method for solving protein structures which cannot be crystallized (Starodub et al *J. Synch Res* 15, 62 (2008)). We have developed a particle injector which provides a single-file beam of hydrated proteins or cells either continuously or on-demand (for synchronization with a free-electron X-ray laser). We are also developing methods for aligning molecules in a beam, including flow alignment, laser alignment and magnetic field alignment. First results will be presented showing ring diffraction patterns from Photosystem I protein crystallites consisting of just 19 x 19 x 21 unit cells, obtained using the coherent undulator beamline 9.0.1 at the Advanced Light Source at 2nm wavelength (Shapiro et al, *J. Synch Rad.* (2008) submitted). Design details of the aerojet gas-focussing droplet beam generator will be given (DePonte et al (2008), Weierstall et al *Expts in Fluids.* (2008)). Radiation damage aspects of diffractive imaging using femtosecond hard X-ray pulses will also be discussed. A solution to the inversion problem of multiple scattering for soft X-rays will be presented. This group effort (see papers for the many contributors) is supported by NSF, CBST, and ARO awards.

Keywords: femtosecond X-rays, serial crystallography, diffractive imaging

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Multi-component solids in crystal engineering

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Multi-component solids have always been studied as an integral part of structural chemistry. The earliest of these substances is perhaps the quinone-hydroquinone donor-acceptor complexes which were identified more than 150 years ago. In the context of recent developments in crystal engineering, the central issue seems to be whether or not there are any fundamental differences between single-component crystals and multi-component crystals with regard to matters such as crystallisation, design principles, structural specificity, propensity towards polymorphism, crystal structure prediction and property tuning. Kitaigorodskii stated that studies of binary crystals of organic substances are a key for studying intermolecular interactions. We have stated that the very isolation of a two-component solid is evidence of the fact that some intermolecular interactions between the different molecules in the solid are more

significant, stronger or more specific than the interactions that are possible between molecules of the same type. Multi-component crystals can have fixed stoichiometries and well-defined structures, or they can be of the substitutional solid solution type. Both varieties are useful in crystal engineering. These themes will be illustrated with examples taken from our research over the years.

Keywords: mixed crystal, co-crystal, hydrogen bond

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From a molecular dating agency to successful co-crystal synthesis

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The crystal structure of a compound, the 3-D orientation and organization of molecules in a highly regular manner, ultimately determines most of the fundamental physical properties of that particular material, e.g. thermal stability, hygroscopicity, conductivity, and mechanical strength. Consequently, an ability to control and change the crystalline environment of both known and unknown compounds (without altering the individual molecular properties) would be of enormous significance to both manufacturers and consumers of solid specialty chemicals such as pharmaceuticals, pigments, energetic materials, toxins, foodstuff, and detergents. The deceptively simple act of molecular recognition, which eventually leads to crystallization, is achieved by balancing a range of relatively weak non-covalent forces, and this presentation will highlight some of our attempts at establishing practical and versatile supramolecular design strategies based on tunable site-specific intermolecular interactions.

Aakeroy, C.B.; Desper, J.; Smith, M.M., *Chem. Commun.* 2007, 3936-3938.

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Aakeroy, C.B.; Salmon, D.J. *CrystEngComm*, 2005, 7, 439-448.

Keywords: co-crystal, hydrogen bonding, halogen bonding

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Multicomponent crystals; Their formation, characterisation and application

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My talk will focus on the role that multicomponent crystals (e.g. solvates, hydrates, cocrystals, salts) play in the design of new organic solids. I will cover mainly applications in the pharmaceutical area, illustrating the various methods of preparing such solids as well as demonstrating some of the resulting benefits. The xanthenes (caffeine, theophylline and theobromine) have been extensively studied within my group and they illustrate many of the important aspects of this area. In addition to describing our experimental