$P2_1$ with $Z = 2$. The molecules are stacking along the b axis(Figs.) to construct two types of water channel structures (I and II) in the dihydrate crystal. The hydrogen bond donor/accepter distances suggest that the channel I forms stronger hydrogen bonds than channel II. Therefore, the first dehydration from dihydrate may occur through the channel II to form the monohydrate crystal without major molecular conformation change. Then the water in channel I may be eliminated with rotation of the phenylethyl substituent of Lisinopril molecule.

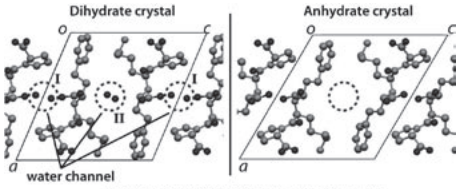

Figure : Crystal structure of Lisinopril

Keywords: powder structure determination, pharmaceutical compounds, crystalline hydrates

MS.80.3

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What do polymorphs teach us about crystal nucleation and growth?

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The ability of a liquid to crystallize as multiple polymorphs is a phenomenon of industrial importance and an opportunity to study crystal nucleation and growth. Using polymorphs to study crystallization follows the tradition of using polymorphs to test principles of thermodynamics and structure-property relations. Part 1 concerns the use of polymorphs to study the nucleation of one crystalline phase on the advancing growth front of another, a phenomenon of interest for controlling crystallization in polymorphic systems. The fastest-nucleating polymorph need not be the product of crystallization, but may nucleate another, faster-growing polymorph. The new polymorph may have higher or lower thermodynamic stability than the initial polymorph. The kinetics of such cross-nucleation were measured and compared with the kinetics of other types of nucleation (primary and growth-front nucleation) in the same liquid. Part 2 concerns the use of polymorphs to study the diffusionless crystal growth that is abruptly activated in certain fragile organic liquids near the glass transition temperature. The phenomenon is important for understanding the stability of amorphous solids. For the ROY system, currently the top system for the number of coexisting polymorphs of solved structures, diffusionless growth exists for some polymorphs but not others, with those showing the growth mode being denser and more isotropically packed.

Keywords: polymorph, crystal growth, nucleation

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Modeling single crystal diffuse scattering on polymorphs of the drug benzocaine

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Understanding and predicting the occurrence of polymorphism is of great importance, particularly for pharmaceuticals. Despite the attention that has been devoted to this problem, progress has been difficult and slow - a fact that may reflect the use of average (Bragg) crystal structures in the development of theoretical approaches. While efforts at crystal structure prediction, including the prediction of polymorphs, have been quite successful for rigid molecules, for conformationally flexible molecules success has been limited [1]. Diffuse X-ray scattering provides information over and above anything that can be learned from conventional crystallography and gives direct information of the local structure of materials and how the atoms and molecules are interacting. The present study is part of a research program in which we are using diffuse scattering methods to probe the local structure and dynamics of molecular systems that exhibit polymorphism, with particular emphasis on pharmaceuticals and molecules with conformational degrees of freedom. We describe a study of the diffuse scattering present in crystals of benzocaine (ethyl 4-aminobenzoate), which is commonly used as a topical local anesthetic. This has two polymorphs: form I is monoclinic $P2_1/c$; form II is orthorhombic $P2_12_12_1$. We have collected three dimensional diffuse X-ray scattering data for the two polymorphs on the 11-ID-B beamline at the Advanced Photon Source (APS). We describe the development of Monte Carlo simulation models used to interpret and analyse these data. Subsequent interrogation of the derived models provides details of the local structure of the two polymorphs and gives insight into the relationship between them.

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Keywords: diffuse scattering, polymorphism, pharmaceuticals

MS.80.5

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Computed crystal energy landscapes as an aid to understanding polymorphism

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The fundamental scientific and industrial interest in controlling crystallisation is inspiring the development of methods of predicting which crystal structures are thermodynamically feasible. Frequently, computing this crystal energy landscape will reveal that there are many crystal structures that are approximately equi-energetic compromises between the various intermolecular interactions allowed by the conformational flexibility. Contrasting these crystal energy landscapes with the solid forms found experimentally shows the capacity to rationalise and predict polymorphism, disorder and a propensity for solvate formation. This will be exemplified by molecules such as uracils, carbamazepine, fluoroisatins, chloronitrobenzenes as well as the subjects of “blind tests”.

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Keywords: crystal structure prediction, organic polymorphism, computed crystal energies

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Crystallography at the new Australian research reactor OPAL

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The newly commissioned 20 MW research reactor OPAL in Australia houses a number of instruments dedicated to crystallography as well instruments for neutron spectroscopy. The initial suite of instruments includes two powder diffractometers and a quasi-Laue single crystal instrument and was selected to reflect the strengths and interests of Australian Scientists. OPAL is characterised by extensive use of state-of-the-art neutron guides that deliver higher fluxes to the instruments. In this presentation I will firstly describe the technical capabilities of these instruments as well that of the closely the allied Small Angle Scattering instrument. Next I shall introduce the scientific capabilities of these instruments demonstrating how the high flux available at the instruments can be utilised either for high-speed or high resolution crystallography.

Keywords: neutron diffraction, international science, diffraction neutrons X-rays electrons

MS.81.2

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Current situation of the cold neutron research facility project at HANARO

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HANARO is the research reactor with 30 MW thermal power with 7 horizotal beam ports and has been operational since its first criticality in 1995. For last 10 years of its early phase, neutron beam instruments of high reolution powder diffractometer, four-circle diffractometer, small angle neutron spectrometer, neutron radiography facility, residual stress instrument, etc.. has been built sequentially around those beam ports using thermal beams. With rapidly increasing demand of cold neutron from continuously expanding users society of universities and industries, the project for the cold neutron research facility construction was launched in July 2003. The project consists of 4 parts; the liquid hydrogen cold moderator and its cooling system utility, the neutron guides, neutron spectrometers and the cold neutron laboratory building. There are 3 relocated neutron spectrometers with modification from the reactor hall and 3 newly developed spectrometers as day-1 instruments. In mid 2008, the cold neutron laboratory will be completed, and tight installation and commissioning schedule for all the four parts of the project is ahead from now to it expected project completion, April 2010. We report in this talk overall project status, schedule, instruments development strategy with users community, and long term prospects.

Keywords: cold neutron spurce, neutron instrumentation, neutron diffraction and scattering

MS.81.3

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SNS and HFIR: Breaking new ground

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The Spallation Neutron Source (SNS) facility became operational in the Spring of 2006, and is now well on its way to become the world-leading facility for neutron scattering. Furthermore, the SNS and the HFIR reactor facility, newly outfitted with a brilliant cold source and guide hall, were brought together within a single Neutron Sciences Directorate at ORNL providing the opportunity to develop science and instrumentation programs which take advantage of the unique characteristics of each source. SNS and HFIR will both operate as scientific user facilities. Access to these facilities is being managed under an integrated proposal system which also includes the Center for Nanophase Materials Sciences (CNMS) and the electron microscopes in the Shared Research Equipment (SHARE) program. Presently SNS has three of the eventual 25 instruments operating in the User program and seven more will begin operations in 2008.
A project to upgrade the power of the SNS accelerator to 3MW is underway and government approval is being sought for construction of a long pulse (1ms) second target station. The future is bright for neutron scattering at Oak Ridge.

Keywords: SNS, HFIR, breaking new ground

MS.81.4

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An advanced pulse neutron source and scientific challenges at J-PARC

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The J-PARC (Japan Proton Accelerator Research Complex) project, which aims at providing world best experimental facilities for condensed matter sciences, elementary particles and nuclear physics, and nuclear transmutation R&D, is now in progress toward its completion. For condensed matter science users, a MW pulsed neutron source will be realized with a number of advanced neutron instruments. The first operation for users is planned to start in December 2008. The MW neutron source with the mercury target system, the cryogenic hydrogen moderator system, and all other