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Guest disorder, clustering and structure of low/high pressure forms of inert gas clathrate hydrates

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Low and high pressure structures of krypton, xenon and argon clathrate hydrates have been studied in situ and in pressure quench recovered forms using high energy (100 keV) synchrotron x-ray scattering (HEXRD) and nuclear magnetic resonance techniques. In addition to standard structural refinements, HEXRD over a wide momentum transfer range has been used to produce Fourier difference maps and pair distribution functions of these structures that indicate the guest electron density. Using relatively simple and higher atomic number inert gas atoms as guests provides enhanced scattering contrast between the guest and the host and allows greater insight into the guest positions and short to intermediate range intercage correlations/disorder of the guest atoms. For krypton hydrate, the low pressure structure II form indicates an enhanced degree of cage-to-cage guest disorder, above that accounted for by ordinary crystalline models. The high pressure hexagonal forms have been produced and successfully quench recovered. The geometry of the large cage guest clusters and intercage guest disorder of this structure are indicated. For the xenon hydrate, we describe the structural refinements for the low pressure structure I form and the in situ high pressure hexagonal form, including descriptions of the guest clustering in the large cages. Structural transformation processes occurring on decompression and recovery of high pressure hexagonal xenon hydrate are also discussed. From the initial low pressure argon hydrate structure I, a filled ice structure is produced above 2.0 GPa, and the structure of this form along with a description of its compressibility is given. ORNL is managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 for the U.S. Department of Energy.

Keywords: high pressure, disordered materials, clathrates

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LaueGUI- an open source Matlab tool for online inspection of time resolved Laue diffraction patterns

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Pink beam Laue diffraction is a powerful tool for determining time-resolved crystallographic structure. The large bandwidth compared to a monochromatic beam allows the simultaneous collection of hundreds of reflections even for moderate size unit cells at fixed orientation. Below 100 X-ray pulses are needed due to the high brightness of the pink beam at a synchrotron. This allows fast data collection and limits sample degradation due to laser excitation. However, there is a large gap between the speed of data collection and the speed of analysis tools. The purpose of LaueGUI is to fill this void by rapidly evaluating time-resolved Laue patterns. The program is based on the use of Precognition (Renz Research), but special care has been taken that the software is self contained in the Matlab environment. LaueGUI is open source written in an object oriented style. It's controlled through a graphical user interface (GUI) and loads free format ASCII files for many configurations. The code was executed with MAR165 and MAR133 (MAR Research) images but other detector image formats can be supported. Successful analysis was completed in a few seconds per image with data from ESRF[1], KEK-AR[2] and APS(BioCARS)[3]. At ESRF data from TTF-CA single crystals were collected using 50 single pulses of the 16 bunch mode at ID09b (U17, 9mm gap, 18keV, 3% bandwidth) that allowed full structure refinement. Comparable data were collected for organometallic samples at KEK-AR using 3-10 single bunches. Download: userpage.chemie.fu-berlin.de/~mcmesser/LaueGUI
references to unpublished data:
[1] M. Messerschmidt, T. Tschentscher, M. Wulff
[2] P. Coppens, M. Gembicky, M. Messerschmidt, M. Pitak, S.-L. Zheng, S.-I. Adachi, S.-Y. Koshihara
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Keywords: time-resolved laue diffraction, crystallographic software development, structural chemistry organic organometallic compou

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A good bye from SMX @ the SRS

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For more than ten years SMX has grown to be one of the most powerful techniques and oversubscribed facilities hosted by the Synchrotron Radiation Source (SRS) located at Daresbury, Warrington. In this final review from the SMX stations I will take a look back over the history of both the SMX Stations, 9.8 and 16.2 SMX, highlighting the many successes and the few failings as SMX hands on the batten to another facility and a new generation of experimenter.

Keywords: synchrotron, non ambient, small molecule

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Phase transition studies for powder and amorphous materials under high pressure

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The study of polymorphism and polyamorphism in pressure domain will undoubtedly broaden our horizons and perspectives of the states of matter in general, and may have a significant impact on the existing theories about the structure, formation, and evolution of crystal and amorphous materials. The zinc oxide from NIST standards was studied under high pressure and low temperature conditions. Metallic glasses were selected to test the pressure induced polyamorphism. The procedure of the pressure-induced amorphous state to crystalline state is another subject in this report. The high