the SCA2Structure pipeline running on a Linux cluster at UGA via the web. The average total time for data collection and structure determination was 191 minutes. The structures solved represented an average mix of structural genomics targets with molecular weights ranging from 12 - 25 kDa. Details of the experiments will be presented. Work supported in part with funds from the NIH (GM62407), The Georgia Research Alliance and The University of Georgia Research Foundation.

[1] Liu, et al., *Acta Cryst*., 2005, D**61**, *in press*.

Keywords: HT structure determination, SCA2 Structure, SER-CAT

MS23.25.4

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The Integration of Data Reduction and Structure Solution - from Diffraction Images to an Initial Model in Minutes

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A new approach that integrates data collection, data reduction, phasing and model building significantly accelerates the process of structure determination and, on average, minimizes the number of data sets and synchrotron time required for a structure solution. The initial testing of the system with 50+ of novel structure determinations proved its high value for MAD/SAD experiments. The heuristics of choosing the best computational strategy for different data resolution limits of phasing signal and crystal diffraction are being optimized. Typical end result is interpretable electron density map with partially built structure and in some cases even almost complete, refined model. The current development is oriented towards a very fast structure solution, in order to provide feedback during the diffraction experiment. Work is also proceeding towards improving the quality of phasing calculation and model building.

Keywords: high throughput structure determination, phasing, model building

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Medium throughput Protein Crystallography: Limiting Steps in the Pipeline

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The **S**tructural **P**roteomics **IN** **E**urope (SPINE) project was the first EC funded structural genomic project. Its aim was to foster the high throughput determination of proteins relevant to human health. The major bottlenecks was recognised to be the expression of soluble and stable proteins in sufficient amounts for crystallization, and this has proved to be true. The pipeline will be briefly summarized and the success rate for a set of proteins described. The presentation will concentrate on a set of targets from *Bacillus anthracis* from the SPINE partner groups in York and Oxford. A number of targets were selected using bioinformatics tools and put through the expression pipeline.

While only a small part of SPINE funds was allocated to crystallographic software, a number of scientists have recently been contributing to automation developments. Recent experience on applying these to SPINE targets will be described and bottlenecks indicated.

Keywords: macromolecules, automation, software

MS24 MOLECULAR CRYSTALS UNDER NON AMBIENT CONDITIONS

Chairpersons: Judith A.K. Howard, Jacqueline Cole

MS24.25.1

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Blowing Hot and Cold and its effect on some crystals

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The benefits of collecting single crystal diffraction data at low temperatures are well known and the use of low temperature devices is now very well established and widespread for small molecule crystallography; in many cases to usefully collect data at a single temperature. The combination of easily controllable devices with a wide temperature range and the use of area detectors allowing rapid data collection makes variable temperature studies and thus exploration of the structural changes that occur with changes in temperature much more accessible.

At the higher end of the temperature scale, and as part of a wider project, we are investigating the effect of temperature on selected porous coordination networks and hydrogen-bonded arrays. These networks, which can be considered metal-organic zeolite analogues, form channels, pores and cavities which may include guest organic molecules. By heating the crystal and collecting data *in situ* we can monitor the structural changes that occur with increased temperature, in particular due to desorption of these guest molecules.

At the lower temperature range we have been investigating structural changes at the metal centre of some transition metal complexes.

Examples from studies carried out in the temperature range 35-500K using an open flow HeliX helium cryostat and a Cryostream plus will be presented.

Keywords: low and high temperature devices, metal-organic compounds, porous materials

MS24.25.2

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Photo-induced Molecular Switching : Neutron Diffraction Studies

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The design of molecules that could be utilized for information storage is one of the main challenge in molecular material science and optical switching is one of the most intense areas of interest in memory molecules. Polarized neutron diffraction (PND) was used for the first time to investigate the photo-magnetic properties of photo-switchable inorganic molecular solids. Spin crossover compounds containing an octahedrally coordinated Fe^{2+} ion present a low spin diamagnetic (S = 0) ground state which can be switched, under light illumination with a suitable light wavelength, to a high spin paramagnetic (S = 2) metastable state having an extremely long lifetime at low temperatures.

A new experimental setup, allowing for both in-situ light illumination and PND measurements, has been developed on the 5C1 diffractometer at the LLB and tested on the $[Fe(ptz)_6](BF_4)_2]$ (ptz = 1-propyltetrazole) spin crossover compound [1]. The photo-excitation kinetics was followed by PND, which evidenced a complete photo-excitation process. The first magnetization density map in a photo-induced magnetic state has been obtained at 2K using a laser beam with 473 nm.

[1] Goujon A., Gillon B., Gukasov A., Jeftic J., Nau Q., Codjovi E., Varret F., *Phys. Rev. B*, 2003, **67**, 220401(R).

Keywords: polarized neutron scattering, molecular magnetism, molecular switches

MS24.25.3

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Photo Excited State Crystallography of Iodo-bridged Dicopper (I) Complex

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Luminescent dicopper(I) complex $[Cu_2I_2(PPh_3)_2(4,4'\text{-bpy})]_\infty$ (bpy=$C_{10}H_8N_2$) consists of $\{Cu_2I_2\}$ planar units, which are bridged by