PS01.05.10 CRYSTAL STRUCTURE DETERMINATION OF BARIUM OXALATE,BaC_2O_4•3.5H_2O/D_2O. A. Norlund Christensen, Department of Inorganic Chemistry, Aarhus University, DK-8000 Aarhus C, Denmark, Reinhard B. Neder, Institute of Crystallography and Mineralogy, University of München, D-80333 München, Germany

The crystal structure of barium oxalate hydrate, BaC_2O_4 3.5H_2O, was solved using synchrotron X-ray powder diffraction data, neutron powder diffraction data of BaC_2O_4 3 5D_2O, and synchrotron X-ray single crystal diffraction data, measured on a microcrystal. The compound is monoclinic, a = 13.489(1), b = 7.663(1), c = 15.085(1) Å, ß = 113.569(5)°, from the neutron data, space group C2/c, No. 15, Z = 4. The precision of the structure arrived at with the synchrotron X-ray single crystal data is higher than that obtained with the neutron powder diffraction data. The barium atoms are bonded to the oxalate ions and to the water molecules with ten barium oxygen bonds in the range 2.704(3) to 2.974(3) Å. The structure has hydrogen bonds in the range 2.732(4) to 2.855(5) Å, and the oxalate ion is planar.

PS01.05.11 ANOMALOUS DISPERSION APPLIED TO A TIN-MORDENITE POWDER SAMPLE AT THE ESRF. A. Frost Jensen*, Centre for Crystallographic Studies, Chemistry Department, University of Copenhagen, Denmark, P. Norby, Chemistry Department, Brookhaven National Laboratory, NY, USA, J.-L. Hodeau, Laboratoire de Cristallographie, CNRS, Grenoble, France, H. Graafsma, A. Kvick, Diffraction Group, ESRF, Grenoble, France, J.-E. Jørgensen, Chemistry Department, University of Aarhus, Denmark

Applications of anomalous dispersion in materials science crystallography is a rapidly developing field, which has benefitted tremendously from the increasing availability and quality of X-ray synchrotron sources in the past decade. At the European Synchrotron Radiation Facility (ESRF), we have at the Materials Science Beamline recorded powder diffractograms of the zeolitic ionic conductor, tin mordenite, at 47 incident photon energies in the range from 29.008 keV to 29.708 keV, bracketing the Sn K- absorption edge at 29.2 keV. The purpose of this study is to determine the Sn atomic positions and the Sn-Sn interatomic distances which cannot be revealed by traditional crystallographic techniques due to a disorder over several sites of the tin ions. (Knudsen, N., Krogh-Andersen, E., Krogh-Andersen, I. G., Norby, P., Skou, E. *Solid St. Ionics.* **61**, (1993), 153). The sample also contains grains of tinoxide, SnO_2, which complicates the analysis, and eliminates a normal EXAFS analysis as a possibility to determine interatomic distances. In order to solve the problem we use the newly developed diffraction anomalous fine structure (DAFS) technique. (Pickering, I. J., Sansone, M., Marsch, J., George, G. N. *J. Am. Chem. Soc.* **115**, (1993), 6302. Stragier, H., Cross, J. O., Rehr, J. J., Sorensen, L. B., Bouldin, C. E., Woicik, J. C. *Phys. Rev. Lett.* **69**, (1992), 3064). This method in principle allows extraction of site-specific absorption spectra, so that despite crystallographic disorder and multiple phases, interatomic distances and valence states of the probe atoms can be determined reliably. We will present the first results of this work.

PS01.05.12 APPLICATIONS OF ENERGY DISPERSIVE DIFFRACTION WITH SYNCHROTRON RADIATION. P. Suortti, V. Honkimäki, European Synchrotron Radiation Facility, B. P. 220, F-38043 Grenoble Cedex, France

The spectral brightness of a high-field wiggler at the ESRF has been determined by using energy dispersive diffraction (EDD) from well-characterized powder specimens. The results are in a close agreement with the brightness calculated from the emittance of the electron beam and the measured magnetic field of the wiggler. The precisely known brightness of the synchrotron beam can be used in many different studies with EDD. In the case of powder diffraction all reflections up to very high orders are recorded simultaneously, and thermal motion parameters are obtained with high accuracy from the integrated intensities. A new method for resolving the powder pattern was developed. Bragg reflections and the background of smoothly varying inelastic scattering and modulated thermal diffuse and disorder scattering are described by a unified and self-consistent model, which is fitted to the observed diffraction pattern. When two samples of different thicknesses are used in transmission geometry the total attenuation coefficient is obtained over a wide energy range. In the case of a single crystal reflection from one set of Bragg planes are recorded simultaneously. The integrated reflectivities are measured on an absolute scale, and this provides a rapid method for determination of the effects of extinction. The energies where the reflections occur are changed by changing the scattering angle, so that the predictions of extinction theories are tested in short order. Results of these applications are presented.

PS01.05.13 STRUCTURE DETERMINATION OF ORGANIC MICROCRYSTAL. Yasuyuki Takenaka, Hokkaido University of Education, Hakodate; Hachiman 1- 2, Hakodate, Hokkaido 040, Japan, Kiyoaki Tanaka and Wakatsu Nagai, Nagoya Institute of Technology; Gokiso, Nagoya 466, Japan, Masaya Uchida, Noboru Suda, and Kazumasa Ohsumi, Photon Factory, National Laboratory for High Energy Physics; Oho 1-1, Tsukuba, Ibaraki 305, Japan

Structure analysis of organic micro-crystal (120x20x20 μm) has been attempted by equi-inclination Weissenberg method with Imaging Plate using synchrotron radiation at BL-4B of Photon Factory in Japan. The equipment was kept in vacuo during data collection. The specimen was a long life time phosphorescent substance in room temperature. The structure analysis is in progress. Data processing for Weissenberg photograph will be also discussed. Crystal data; P -4 21 c (No. 114), a = b = 20.19 Å, c = 7.70 Å, α=ß=γ= 90, V = 3139 Å^3, λ= 1.198 Å, 1114 reflexions of which 283 independent, -12 <= h <= 18, -11 <= k <= 19, 0 <= l <= 5.

Detectors & Data Processing II

MS01.06.01 THE PERFORMANCE OF X-RAY DETECTORS BASED ON IMAGE PLATES. M. Thoms, R. Fasbender, N. Gloser, A. Kinne, A. Winnacker, University of Erlangen-Nürnberg, Institute for Material Science VI, Martensstr. 7, 91058 Erlangen, Germany

X-ray detectors, which are based on image plates are increasingly used in crystallography. The performance of these detectors and therewith the quality of the acquired data depends on two basic processes: The conversion of x-ray radiation into storage centers and the readout of the stored information. Both processes are influenced by characteristics of the image plate and the reader as well. These characteristics are for instance the thickness of the phosphor layer, the type of phosphor and its grain size, the laser intensity and the sensitivity of the utilized photodetector in the reader. The effect of these parameters on the image resolution, the noise of the image and the quantum efficiency of the detector and therewith on the quality of the data will be discussed.

It will be shown by examples, that a spatial resolution of 50μm, a precision of the dose measurement better than 1% and an acquisition time of less than 40s for an image of 20x30cm^2 consisting of 17.5 million pixels can be reached in the case of an optimized detector.