the framework occurs upon calcinations, thus explaining the negative thermal expansion.

[1] D. Taylor, *Mineralogical Magazine* **1968**, *36*, 761-769. [2] M. Antao, I. Hassan, J. B. Parise, *The Canadian Mineralogist* **2004**, *42*, 1047-1056. [3] I. Hassan, S.M. Antao, J.B. Parise, *American Mineralogist* **2004**, *89*, 359-364. [4] Z. Zheng, V.V. Guliants, S. Misture, *Journal of Porous Materials* **2009**, *16*, 343-347.

Keywords: negative thermal expansion, trioxane silica sodalite, in situ time-resolved diffraction.

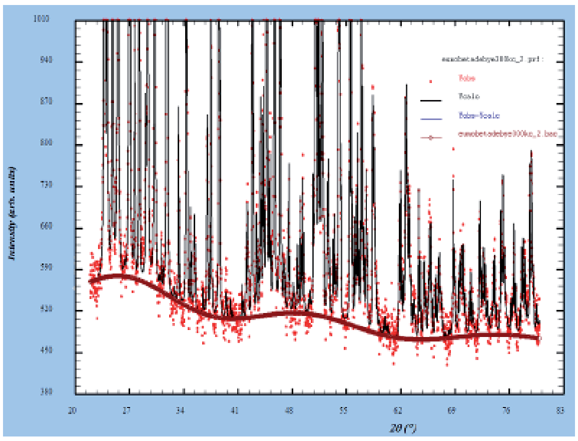
MS05.P29

Acta Cryst. (2011) A**67**, C249

Structural study of $Eu_2(MoO_4)_3$ and $Sm_2(MoO_4)_3$ polymorphs

C. González-Silgo,[a] M. C. Guzmán-Afonso,[b] M. E. Torres,[c] J. González-Platas,[a] E. Matesanz,[d] M. Castro,[e] Ulises R. Rodríguez-Mendoza[b] [a]*Departamento de Física Fundamental II,* [b]*Departamento de Física Fundamental y Experimental, Electrónica y Sistemas,* [c]*Departamento de Física Básica, Universidad de La Laguna, La Laguna, S/C Tenerife (Spain).* [d]*C.A.I. Difracción de Rayos X, Universidad Complutense de Madrid, Madrid (Spain).* [e]*Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, Zaragoza (Spain).* E-mail: csilgo@ull.es

Light RE molybdates (RE=La-Eu) can occur in two differently ordered scheelite-type ($CaWO_4$) structures: $La_2(MoO_4)_3$ [1] and α-$Eu_2(MoO_4)_3$ [2]. Intermediate molybdates (RE=Sm-Ho) show the β'-$Gd_2(MoO_4)_3$ ferroelectric-ferroelastic phase [3]. A sound knowledge of the dielectrical and optical properties of $RE_2(MoO_4)_3$ crystals correlated with their crystal structure is of fundamental importance for the application of these materials. Sm and Eu molybdates are particularly interesting because both phases (α and β') are stable at room conditions [4], [5]. In this work, we have studied the evolution of the four phases (α, β', β and amorphous) of $Eu_2(MoO_4)_3$ and $Sm_2(MoO_4)_3$ with the temperature, in order to explain a new anomaly detected in their dielectric permittivity and in the heat capacity around 275K. Such anomaly can be related with a phase transition between the ferroelectric phase β' and/or to the α phase, before the ferroelectric(β')-paraelectric(β) transition and the β-α transition at higher temperature. We have applied a new alternative method for treating distorted structures by means of symmetry mode analysis, performed using the program AMPLIMODES, developed in the Bilbao Crystallographic Server [6], and the Rietveld refinement of the amplitudes of such symmetry modes, instead of dealing with the atomic coordinates using the Fullprof program [7]. Moreover, the diffuse scattering has been analyzed and quantified to explain the dielectric and thermal anomalies.



[1] W. Jeitschko *Acta Cryst.* **1973**, *B29*, 2074. [2] K. Boulahya, M. Parras, J.M. González-Calbet, *Eur. J. Inorg. Chem*. **2005**, *967*. [3] H. Nishsiska, W. Odajima, M. Tateno, K. Ueda, A.A. Kaminskii, A.V. Butashin, S.M. Bagayev, A.A. Parilink. *Appl. Phys. Lett*. **1997**, *70*, 1366. [4] M.C. Guzmán-Afonso, M.E. Torres, N. Sabalisck, C. González-Silgo, J. González Platas, A. Mújica, E. Matesanz, Send to *Solid State Comm* **2011**. [5] C. Guzmán-Afonso, C. González-Silgo, M.E. Torres, N. Sabalisck, A.D. Lozano-Gorrín, J. González-Platas, E. Matesanz, Send to *Materials Letters*. **2011**. [6] D. Orobengoa, C. Capillas, M.I. Aroyo, J.M. Perez-Mato, *J. Appl. Cryst*. **2009**, *A 42*, 820. [7] J. Rodríguez-Carvajal, Physica B. **1993**, *192*, 55.

Keywords: rare-earth molybdate, phase transition, polymorphism.

MS05.P30

Acta Cryst. (2011) A**67**, C249

Recent developments at the ECHIDNA high-resolution neutron powder diffractometer

Maxim Avdeev, James Hester, *Bragg Institute, ANSTO, Sydney, (Australia).* Email:max@ansto.gov.au

The ECHIDNA high-resolution neutron powder diffractometer at OPAL has been in routine and largely trouble-free operation for three years. Data from ECHIDNA have appeared in over 30 publications, covering a temperature range of 1.5K to 1900K and magnetic fields up to 7 T.

ECHIDNA data reduction is largely automated, with a user-friendly interface and a wide choice of output formats (hdf, pdCIF, xyd, GSAS). Data reduction implements a sophisticated approach to gain correction, described in a companion poster [1], and provides large amounts of metadata relating to the data reduction via the pdCIF output format.

The range of instrument configurations continues to expand. A low-temperature (<1K), cryogen-free top-loading cryostat is currently being commissioned and first results are reported. In addition, the maximum takeoff angle has been increased from 140 to 155 degrees without compromising our ability to use the robotic sample loader.

In addition to the regular calls for proposals twice a year, ECHIDNA operates a popular fast access mail-in program. In order to participate, applicants should fill in the simple web-based form accessed via http://neutron.ansto.gov.au. Following safety and technical review, applicants forward their samples to us and data are returned typically within one month of sample receipt. Mail-in sample environment is usually restricted to room temperature and/or 4K.

[1] J.R. Hester, *"Efficiency correction for neutron powder diffraction area detectors",* MS-68

Keywords: powder diffraction, instrumentation, neutron

MS05.P31

Acta Cryst. (2011) A**67**, C249-C250

High-Pressure Neutron Diffraction Study of $Fe_{1.087}Te$

Jens-Erik Jørgensen, *Department of Chemistry, University of Aarhus, DK-8000 Aarhus C (Denmark).* E-mail: jenserik@chem.au.dk

The crystal and magnetic structures of $Fe_{1.087}Te$ were studied at high pressures and low temperatures. The experiment was performed on the DMC diffractometer at the SINQ spallation source at Paul Scherrer Institut, Switzerland. The sample was loaded into a clamp type pressure-cell using Fluorinert as the pressure transmitting medium. NaCl was used as an internal standard for pressure calibration and the