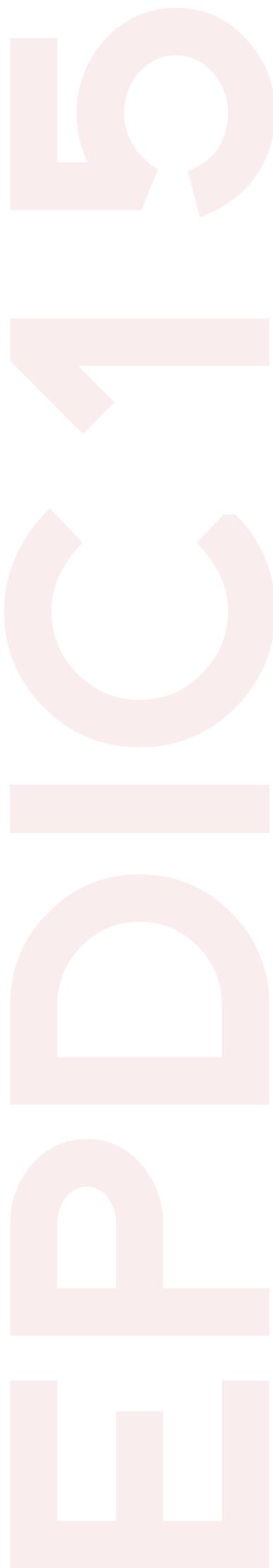


EPDIC 15

The European
Powder Diffraction
Conference

Bari, Italy, 12-15 June 2016
The Nicolaus Hotel

BOOK OF ABSTRACTS



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MS12 - High pressure diffraction

Chairs: *W. Paszkowicz* (University of Warsaw, Poland)

G. D. Gatta (University of Milan, Italy)

Microsymposium: Wednesday, June 15, Afternoon

Poster session: Tuesday, June 14, Afternoon

POSTERS

MS12-P01 Crystal-fluids interaction in zeolites at high pressureD. Comboni^a, P. Lotti^b, G. D. Gatta^{a,c}^a*Dipartimento di Scienze della Terra, Università degli Studi di Milano, Italy*^b*Elettra - Sincrotrone Trieste S.c.P.A., Italy*^c*CNR - Istituto di Cristallografia, Bari, Italy*

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Zeolites (natural or synthetic) are a class of open-framework silicates with cavities, in the form of channels or cages, with diameters shorter than 2 nm. These porous materials respond to the applied pressure differently, in response to the nature of the pressure-transmitting fluids, used to compress hydrostatically the materials under investigation. For instance, cavities can be accessed or filled by suitable guest chemicals, intruded in the zeolitic pores upon compression. Moreover, pressure can play an important role also in increasing the efficiency of zeolites as "nano-reactors", favoring the access of reactants and products to/from the catalytically active sites and the aggregation of molecules in the cavities. Over the last years [1,2,3], we have performed a series of experiments - by *in-situ* single-crystal and powder synchrotron diffraction using a number of penetrating and non-penetrating pressure transmitting fluids with a diamond anvil cell - in order to describe the crystal-fluid interaction upon pressure of a series of natural or synthetic zeolites with different topologies and compositions, expected to favor or not the penetration of liophilic/hydrophobic guest species. The following aspects were investigated: 1) the structural deformations of the tetrahedral framework in response to the isotropic compression regime; 2) the unit-cell variations with pressure and the elastic anisotropy; 3) the penetration of molecules of the *P*-fluid (*e.g.*, H₂O, methanol, ethanol, ethylene glycol), along with the host-guest and guest-guest interactions; 4) the reversibility extents of the observed phenomena.

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[1] Gatta G.D. *Microporous and Mesoporous Materials*, 2010, 128, 78. [2] Gatta G.D., Lee Y. *Mineralogical Magazine*, 2014, 78, 267. [3] Lotti P., Arletti R., Gatta G.D., Quartieri S., Vezzalini G., Merlini M., Dmitriev V., Hanfland M. *Microporous and Mesoporous Materials*, 2015, 218, 42.

Keywords: zeolites, high pressure, crystal-fluid interaction

MS12-P02 High-pressure X-ray diffraction study of GaF₃J.-E. Jørgensen^a, Y. Filinchuk^b, V. Dmitriev^c^a*Department of Chemistry, Aarhus University, Denmark*^b*Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Place L. Pasteur, B-1348, Louvain-la-Neuve, Belgium*^c*Swiss-Norwegian Beam Lines, European Synchrotron Radiation Facilities, BP 220, F-38043 Grenoble Cedex, France*

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The VF₃-type compounds GaF₃ have been studied by high-pressure angle dispersive X-ray diffraction in the pressure range from ambient to 10 GPa. Rietveld refinements of the measured data sets were performed in space group R-3c using hexagonal setting. The compression mechanism was found to be highly anisotropic. The *c*-axis shows little pressure dependence ($\approx 0.5\%$) but exhibits negative linear compressibility up to ≈ 3 GPa where it achieves its maximum value. In contrast the *a*-axis is reduced by $\approx 9\%$ at the highest measured pressure and an anomalous reduction in the linear compressibility is observed at 4 GPa. The volume reduction of GaF₃ is mainly achieved through coupled rotations of the GaF₆ octahedra around the *c*-axis, which reduces the length of the *a*-axis while the GaF₆ octahedra remain almost non-distorted. The compression mechanism of GaF₃ will be discussed in terms of deformation of an 8/3/c2 sphere-packing model as well as illustrated by changes in void space volumes [1,2]. The zero pressure bulk modulus B_0 and its pressure derivative B_0' were determined to $B_0 = 27(3)$ GPa and $B_0' = 5.6(10)$. The relationship between zero pressure bulk modulus and unit cell volumes will be discussed for GaF₃ and MF₃ compounds where M is a first-row transition-metal.