

MS20-P16 Pressure-induced penetration of organic molecules in Si-Ferrierite

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In the last 10-15 years, the behavior of natural and synthetic zeolites under pressure has attracted great attention (i.e. [1,2]). These porous materials respond to pressure in a large variety of modes and the effects of applied pressure and molecular spatial confinements of the pressure transmitting media can open extremely interesting applicative scenarios. For instance, owing to their open framework with cages and channels of molecular dimensions, zeolites could be considered as a negative-image of nanomaterials: the relevant nanosized portion is the open space which can be accessed or filled by suitable guest chemicals, intruded in the zeolite pores upon compression. Moreover, pressure can play an important role also in increasing the efficiency of zeolites as "nano-reactors" in the field of heterogeneous catalysis, favoring the access of reactants and products to/from the catalytically active sites and the aggregation of molecules of proper shape in the microporous cavities. In this study we explore - by both single-crystal and synchrotron X-ray powder diffraction and using a number of penetrating and non-penetrating pressure transmitting media - the crystal-fluid interaction upon pressure of a siliceous matrix with ferrierite-type topology [Si-FER: Si₃₆O₇₂], expected to favor the penetration of liophilic/hydrophobic guest species. The following aspects are investigated: *i*) the structural deformations induced by compression on the framework; *ii*) the elastic parameters and the unit-cell variations in response to pressure; *iii*) the penetration of extraframework H₂O and/or organic guest molecules (methanol, ethanol, ethylene glycol, 2methyl-2propen-1-ol); *iv*) the reversibility extents of the observed phenomena; *v*) the comparison between the overall elastic behavior of Si-FER and those of other siliceous zeolites.

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MS20-P17 Crystal structure mechanism of the hydrostatic compression in Mg-rich orthopyroxene

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Orthopyroxene is supposed to make 10 – 20% of the Earth's material under the Lithosphere and thus represent one of the major minerals of the uppermost Mantle. Its high-pressure stability is rather limited compared to other mantle minerals and terminates at around 300 km depth. That orthopyroxene might be one of the crucial factors in the formation of Asthenosphere (magma-generating layer at the bottom of Lithosphere) was suggested from a study of water solubility in this mineral [1]. Recent accurate studies of the crystal structure of pure enstatite [2] and of the Al+H-rich enstatite (this work) contribute high-pressure crystal structure data which, in combination with previous accurate studies of Ca-rich [3] and Fe+Al-rich [4] enstatite give possibility to investigate influences of various expected natural substitutions in the Mg end-member of the orthopyroxene solid solution. All studies were made with the use of improved diamond-anvil cells on laboratory diffractometers with area detectors. Details of the development of crystal structures under hydrostatic compression explain the destabilization of Ca-substituted orthopyroxene on high pressures and the opposite effect of the Fe+Al or Al+H substitution. They are illustrated through detailed analysis of the bond lengths, polyhedral volumes and polyhedral distortions of the four distinct coordination polyhedra in this crystal structure. [1] Mierdel, K., Keppler, H., Smyth, J.R., and Langenhorst, F.: *Science*, 315, 364–368 (2007). [2] Periotto, B., Balić-Žunić, T., Nestola, F., Katerinopoulou, A., Angel, R.J.: *American Mineralogist*, 97, 1741–1748 (2012). [3] Nestola, F., Gatta, G.D., and Boffa Ballaran, T.: *American Mineralogist*, 91, 809–815 (2006). [4] Nestola, F., Boffa Ballaran, T., Balić-Žunić, T., Secco, L., and Dal Negro, A.: *American Mineralogist*, 93, 644–652 (2008).

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