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ABSTRACT BOOK

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COVER IMAGE:

Aerial cityscape image of Turin during sunset.

Pressure-driven methanol intrusion in MFI-zeolites and its effects on the structural deformation in silicalite-1

Pagliaro F.*[1], Comboni D.[2], Battiston T.[1], Gatta G.D.[1] & Lotti P.[1]

[1] Dipartimento di Scienze della Terra "A. Desio", Università di Milano. [2] ESRF, Grenoble (France).

Corresponding author e-mail: francesco.pagliaro@unimi.it

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The crystal structure of MFI-zeolites is characterized by SiO_4 interconnected tetrahedra, which define two major structural channel systems, confined by 10-members rings (10mRs) of tetrahedra running along [010] and sinusoidal cavities along the [100] direction. The MFI-type zeolites are currently used in methanol-to-olefins (MTO) production processes as catalysts, representing an alternative to the high energy-demanding Steam Cracking process, which accounts for 95% of the worldwide olefins production. Under ambient conditions, only the surfaces of the crystallites are supposed to be involved in the MTO processes. Applying a hydrostatic pressure could significantly increase the efficiency of the catalytic process, enhancing the injection of the methanol molecules through the zeolitic channels. In this light, we aimed to study the influence of pressure to improve methanol capability to enter the structural voids of MFI zeolites. For this purpose, six MFI-type zeolites, characterized by slight chemical differences pertaining Fe-, Al- and B-abundance in the siliceous frameworks, balanced by Na^+ or H^+ as extra-framework cations, have been synthesized. The compressional behavior of these zeolites has been studied by means of *in situ* powder X-ray diffraction up to 2 GPa. A diamond anvil cell (DAC) has been used as a device to generate pressure and both penetrating and non-penetrating fluids have been used as pressure-transmitting media: methanol (able to penetrate the structural voids of the MFI zeolite) and silicone-oil (a polymeric fluid with a kinetic diameter of the molecules larger than the diameters of the structural channels). A different compressional behavior was observed, as a consequence of the intrusion of methanol within the MFI structural channels. The difference in compressibility of the same zeolite sample in silicone oil and methanol has been used as a parameter to evaluate the efficiency of the intrusion process. A comparative analysis of the effect of pressure on the methanol adsorption by the MFI zeolites with different chemical composition may provide useful information on their application as catalysts in the methanol-to-olefins conversion processes. It has been observed that zeolites with higher Fe contents and silicalite-1 (i.e., the 'pure' SiO_2 polymorph with a MFI topology) are the least compressible zeolites in methanol (with respect to silicone oil) and, consequently, those with the highest capability to host methanol molecules within their structure.