

Combined XRPD and Spectroscopic Study of Molecules Hosted in Zeolitic Channels

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Zeolites are tridimensional organized microporous systems hosting positively charged cations balancing the negative charge of the framework and acting as strong Lewis acid centres. Such materials play a great role in industrial chemistry, as they are very efficient catalysts exhibiting remarkable shape selectivity. The pore dimension and topology select the reactants molecules able to penetrate the framework and to reach the internal active sites. The same holds for the intermediate molecules formed on the sites and for the final products able to leave the zeolite framework that actually acts as a nanoreactor of molecular dimension. The understanding of the site reactivity can be achieved by comparing the cations position in the activated catalyst (zeolites subjected to thermal treatments in vacuo conditions, exhibiting no molecules in the channels) with that occupied upon interaction with selected molecules dosed in situ either from the gas or from the liquid phases. The combination of high resolution XRPD data (collected in situ at the ID31 instrument of the ESRF) with XAFS, IR and Raman spectroscopies is a complete approach to face this complex problem, see e.g. [1-3].

[1] Marra G. L. et al., *J. Phys. Chem. B*, 1997, **101**, 10653. [2] Turnes Palomino G. et al., *J. Phys. Chem. B*, 2000, **104**, 8641. [3] Lamberti C. et al., *Nucl. Instr. Meth. B*, 2003, **200**, 155.

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