



XANES-PCA analysis of Ti-species in MCM-41 mesoporous silica synthesized by different methods

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ABSTRACT

MCM-41 mesoporous silica was prepared with Ti incorporated in the structure by two different ways: hydrothermal and atmospheric pressure by sol–gel method. To evaluate each synthesis, these materials were in situ investigated through X-ray absorption fine structure (XAFS) spectroscopy in different stages of the synthesis. X-ray absorption structure at the near edge region (XANES) gives the coordination of Ti and the relative concentration of Ti-species present in the mesoporous materials, obtained by different synthesis. The Principal Component Analysis (PCA) of XANES spectra indicate that mesoporous silica modified by Ti synthesized by hydrothermal method has species with majority of Ti tetrahedrally coordinated. This coordination is increased up to six when the sample is hydrated. In the case of the sol–gel synthesis, Ti-sites have higher mean coordination, independently from the degree of hydration.