

# Effect of calcination parameters on structural properties of Ti-MCM-41 materials synthesized at room temperature (p1103000325.doc)

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Ordered mesoporous materials have stimulated great interest in the scientific community in the fields of catalysis and materials science since their disclosure in 1992. The most important features for their use in catalysis are the extremely high surface area, which potentially allows an efficient dispersion of active sites, and the large and uniform pore diameters in the mesopore range that favour the diffusion of bulky molecules. However, the introduction of the heteroatoms into ordered mesoporous silicas to make them catalytically active can lead to a decrease in the quality of the pore structure as compared with the pure silica grades, the extent of which may depend on the preparation and calcination conditions. In this work is presented a study of the effect of calcination parameters namely, heating rate, calcination temperature, total calcination time and time at final temperature, on pore structural properties of Ti-MCM-41 materials. The materials were prepared by direct synthesis at ambient temperature and pressure, using tetraethoxysilane, titanium alcoxides, cationic surfactants and ammonia, as previously described and were characterised by X-ray diffraction, nitrogen adsorption at 77K and DR UV-Vis absorption spectroscopy. The Si/Ti values of the final calcined materials were determined by AA (Si) and ICP (Ti). The results of this study show that this method allows the preparation in a short period of time of well structured Ti-MCM-41 materials with high thermal and mechanical stabilities without necessity of external heat or pressure. Furthermore the similarity in the Si/Ti values of the synthesis gel and final calcined materials denotes an optimal compromise between synthesis performance and synthesis costs. On the other hand it can also be conclude that a heating rate of  $3\text{Kmin}^{-1}$  and a calcination period of 15h at  $550^\circ\text{C}$  provide middle term calcination parameters which are economically reasonable and do not affect the structural quality of Ti-MCM-41 materials.

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