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DIRECTING FACTORS AFFECTING THE SYNTHESIS OF A MFI-TYPE ZEOLITE

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Zeolites are crystalline tectosilicates constituted by (TO₄) tetrahedra connected through the oxygens of their vertices. The importance of these materials is that their properties differ, due to their variable compositions and structures, leading to the possibility of applying them into different industries, for example, as catalyst in petroleum industry or sensors in quality control. One of the big questions in this area is about the understanding of the chemistry that directs to one or another type of zeolite. Another important question is the search of new zeolitic structures for new applications. One approach to answer both is the study of the structure-directing agents, which are inorganic or organic molecules used in the synthesis of zeolites. New and already-used molecules have been studied within different synthesis conditions and different techniques, as characterization or computational studies. And several attempts of rationalization were and, still, will be performed. In this research, an imidazolium-based compound was studied in hydrothermal zeolite synthesis as organic structure-directing agent (OSDA). The products were obtained with Si/Al or Si/(Al+Zn) compositions, proved by ICP data. X-ray diffractograms showed two different zeolitic types: MFI and TON. It was observed that when Zn was present in the synthesis gel, pure MFI phases were able to appear. But in his absence, the products were all mixtures of MFI and TON zeolites. It was also possible to distinguish both phases by SEM micrographs, as MFI had brick-like shape and TON appeared as needles. The obtained zeolites were stable until 900°C minimum, as tested by a TG/DTG/DSC experiment. To prove that the chosen OSDA directed these structures, a CHN analysis was performed, resulting in integrity of the molecules inside the zeolitic pores and cavities. Finally, a rationale about the location and conformation of the OSDA was needed to understand these experimental results. So, it was done systematic computational calculi that resulted in three different possible locations and four different possible conformations, selecting them for their lower energy related to high stability.