Investigation on the Beckmann rearrangement reaction using B-containing zeolites as catalysts by solid state NMR and theoretical calculations

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Beckmann rearrangement of ketoximes into amides has been extensively studied for many years because their industrial applications, being the conversion of cyclohexanone oxime into ε-caprolactam, the precursor of Nylon-6, one of the most important. Much effort has been done to develop solid catalysts to substitute the classical sulphuric acid, making the process heterogeneous and environmentally friendly [1-3], being zeolites among the most investigated catalysts

During the last decade, Hölderich and co-workers reported the excellent catalytic performance of B-containing zeolites. These authors investigated the influence of boron removal by postsynthesis modifications, e. g. calcinations, acid/base treatment, and concluded that this leads to significant activity and selectivity losses [4, 5, 6].

Here, the combination theoretical calculations of ^{15}N chemical shifts and in situ solid state NMR spectroscopy have been applied to investigate the Beckmann rearrangement reaction over B-containing zeolites, studying the nature of the reaction intermediates and the interaction of the organic molecules with the zeolite framework. ^{1}H to ^{15}N CP/MAS and ^{11}B MAS and MQMAS experiments were measured in order to clarify the interactions above mentioned. The results obtained help to understand the previous catalytic results.

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