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Solid state NMR spectroscopy: a tool for the investigation of zeolites as catalysts and adsorbents

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Solid state nuclear magnetic resonance spectroscopy (ss-NMR) is a very powerful technique for the investigation of all kind of solid materials, including pharmaceuticals, soils, organics, polymers, cements, ceramics or batteries among others. NMR spectroscopy provides evidence at an atomic level on the local environment of the nuclei difficult to obtain by other techniques.
Ss-NMR has been largely used in the investigation of zeolites, which are crystalline microporous silicate or aluminosilicate-based materials with a three-dimensional structure with channels and cavities of molecular dimensions. The unique properties of zeolites are responsible of their application as catalysts in petrochemical and chemical industry and as adsorbents in separation processes. Relevant information on zeolites and their applications that can be obtained by ss NMR will be illustrated here with three case studies:

1.- Structural characterization of RTH type zeolite provides very valuable information for the elucidation of the 3D structure. Zeolites are synthesized using organic molecules as structure directing agents (OSDA) and very often in fluoride medium. The information obtained by combining 19F, 13C and 29Si NMR spectroscopy is essential to determine the structure and the distribution of the atoms in the solid. Moreover, application of 2D 1H NMR pulse sequences will be used to determine the number of silanol groups involved in structural defects.

2.- The investigation on the mechanism of the Beckmann rearrangement reaction of oximes into amides on zeolite catalysts. The use of 15N-ss NMR in combination with DFT calculation allowed to establish that the reaction intermediates formed is different on zeolites containing Brønsted acid sites or silanol defect groups.

3.- Pulse field gradient (PFG) NMR spectroscopy is used to obtain information on the diffusion of small hydrocarbon molecules within the zeolites pores as this process plays a key role on their applications in gas separation and catalysis. This technique has been allowed to stablish that the diffusion of alkene (ethene, propene) molecules within the pores of the microporous silico-aluminophosphate SAPO-34 is promoted by the presence of Brønsted acid sites, while these sites have no influence on the transport of alkanes.

Primary authors: Dr BLASCO, Teresa (Instituto de Tecnología Química (UPV-CSIC)); Dr BLASCO, Teresa

Presenter: Dr BLASCO, Teresa (Instituto de Tecnología Química (UPV-CSIC))

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