17 IZC, 2013. ORAL COMMUNICATIONS

O-2.3-01

Key Molecular Mechanisms for Zeolite Formation

<u>M. Castro¹</u>, W. Park², M. Houas³, G. Brabants⁴, E. Breynaert⁴, I. Lim¹, C. Kirschhock⁴, F. Taulelle³, R. Ryoo⁵, F. Schüth¹, W. Schmidt¹

¹Max-Plank-Institut für Kohlenforschung, Mülheim a.d. Ruhr, Germany, <u>castro@kofo.mpg.de</u>

²Department of Chemistry, KAIST, Daejeon 305-701, Korea

³Tectospin, University of Versailles Saint Quentin en Yvelines, France

⁴Center for Surface Science and Catalysis, K. U. Leuven, Belgium

⁵Center for Nanomaterials and Chemical Reactions, Institute for Basic Science, Daejeon 305-701, Korea

Zeolites are highly valuable materials for industrial applications, especially for catalytic processes and as adsorbents. Nevertheless, the molecular mechanisms involved in their formation remain poorly understood and therefore, the synthesis of zeolites continues on an empirical stage. Our research aims to identify the key mechanisms on a molecular scale with the goal of understanding the factors that drive the formation of zeolites. Here, we report the first study of the molecular mechanisms involved in the formation of microporous and mesostructured zeolite beta from liquid phase using electrospray ionization mass spectrometry (ESI-MS), ²⁹Si and ²⁷Al liquid-NMR spectrometry, DOSY NMR (diffusion experiments) and small angle X-ray scattering (SAXS).

O-2.3-02

At-line analysis of the crystallization of Zeolite LTA by Raman spectroscopy

T.F. Chaves¹, F.L.F. Soares², <u>**R.L. Carneiro**^{2*}</u>, D. Cardoso¹ ¹Dep. of Chemical Engineering, Federal University of São Carlos, São Carlos, Brazil. ²Dep. of Chemistry, Federal University of São Carlos, São Carlos, Brazil. <u>*renato.lajarim@ufscar.br</u>

Several studies have been directed to comprehend the mechanism involved in the production of zeolites. The use of Raman spectroscopy has been shown to be an important technique for the understanding of its catalytic mechanisms and syntheses. In this work the synthesis of zeolite LTA was monitored by Raman spectroscopy, using a reaction mixture with high alkalinity. The synthesis was carried out at 25 °C and Raman spectra were collected at different reaction times, from the liquid and solid phases during 80h of reaction. During the reaction, some spectra of the liquid phase had shown bands centered at 618 cm^{-1} and 1066 cm^{-1} , which are attributed to the soluble hydrated aluminosilicate species and $CO_3^{2^\circ}$ species formed in the gel due to the capture of atmospheric CO_2 by the highly alkaline mixture. After 56 h it was possible to observe a better definition of the band at 500 cm⁻¹, which is related to the presence of the characteristic four-membered rings (4R) of this zeolite. The LTA zeolite was successfully synthesized after 72 h of reaction. DRX analyses of solid products at 24, 48, 72 and 80h of reaction time confirmed that there were not crystalline forms until 48h of reaction, what confirms the data obtained by at-line Raman analysis.