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Solid state NMR studies of ethylene/Ag-zeolites systems

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Ethylene is an important raw material for the production of wide variety of polymers. However, this gas usually appears mixed with other components, as for instance ethane and purification to a single component is required. Nevertheless, the separation of these gases, which have similar properties, sizes and molecular structures is still challenging. In the case of ethylene, its separation using Ag-zeolites is possible due to the selective interaction between ethylene and silver located in zeolite structure (π-complexation). In fact, high stability of the π-complex prevents the participation of ethylene in aromatization reaction on Ag-containing zeolites at high temperatures. [1-3]

The aim of this work is the characterization of the silver species formed in chabazite zeolite (CHA), depending on the degree of hydration and after adsorption of ethylene.

CHA zeolite with a Si/Al =5 molar ratio was synthetized by hydrothermal method and then, Ag-CHA was prepared by ion exchange using a 0.3M AgNO3 solution obtaining a silver content 11 wt%. Ethylene adsorbed on the sample degassed at 400ºC during in an amount equivalent to one molecule of ethylene per unit cell.
UV-Vis analysis of as-prepared sample presents a main signal at 211 nm corresponding to dispersed Ag+, while the evacuated material shows signals at 283 and 317 nm indicating that most silver is forming clusters (Agmδ+). One more signal is also noted at 404 nm, corresponding to metallic silver nanoparticles. The 109Ag solid state NMR spectrum shows a signal at 30 ppm in the as-prepared sample, assigned to Ag+. In contrast, the spectrum of dehydrated sample presents a peak at 5256 ppm, corresponding to Ag0. A priori the cationic silver signal is not observed, as indicated by UV-Vis, so the possibility of paramagnetic silver species is an idea to consider because the presence of these species may affect the relaxation time of the nucleus under study. After that, the presence of paramagnetic species is confirmed by Electron Paramagnetic Resonance (EPR) with high intensity signal with g = 2.003.
In addition, the 13C NMR spectrum recorded after the adsorption of ethylene shows a broad signal at 110 ppm, while ethylene gas appears at 120 ppm. In the case of 109Ag NMR spectrum, a signal at 5284 ppm is observed. These changes in the chemical shift of signals at both 13C and 109Ag NMR proves the ethylene-silver interaction.

In conclusion, the interaction between silver and ethylene is observable by solid-state NMR spectroscopy. The presence of paramagnetic silver clusters in the dehydrated sample is demonstrated by UV-Vis and EPR studies.

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