Use of alkylarsonium cations as probe molecules for the study of zeolites

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Zeolites are crystalline microporous materials of great interest not only from an academic point of view but also from an industrial point of view due to their properties and multiple applications. These properties largely depend on its chemical composition but also on its structure. At present, the International Zeolite Association (IZA) has accepted 242 different structures [1], each with specific characteristics and a particular crystal structure. Obtaining one or the other structure is highly influenced by the organic structure directing agents (OSDAs) used during the synthesis.

Although the most typical OSDAs consist of alkylammonium cations, molecules containing phosphorous or sulfur atoms instead of nitrogen have also been described in recent years. Recently, our group also described the use of alkylarsonium cations, where nitrogen is replaced by an arsenic atom, which effectively lead to the formation of a zeolitic structure [2].

The use of As in ADE provides some additional benefits, since it allows the incorporation of heavy atoms that can act as a probe for different studies of the materials obtained. Its high electron density, compared to that of nitrogen, allows its easy location even using laboratory X-ray powder diffraction equipment; to date, the location of alkylammonium cations often requires the use of single crystal techniques or the use of complex methods. Furthermore, this substitution of N for As allows the use of other advanced characterization techniques, such as nuclear magnetic resonance MAS-NMR of ⁷⁵As in the solid sample, or X-ray absorption spectroscopy (XAS) at the K border of As, to analyze the location and properties of the molecule within the zeolitic network and its evolution under non-standard conditions.

[1] http://www.iza-structure.org/databases/

[2] Sáez - Ferre S., Lopes Ch.W., Simancas J., Vidal - Moya A., Blasco T., Agostini G., Mínguez Espallargas G., Jordá JL, Rey F. and Oña - Burgos P. (2019) Use of Alkylarsonium Directing Agents for the Synthesis and Study of Zeolites. Chemistry - A European Journal 25, 16390-16396

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