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ITQ-52, a new microporous zeolite with interconnected small and medium pores obtained using an aminophosphonium dication as structure directing agent

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Zeolites are usually obtained using tetraalkylammonium cations as organic structure directing agents (OSDAs). Recently, we have reported the synthesis of new zeolites using tetraalkylphosphonium (ITQ-26, ITQ-27, ITQ-34, ITQ-49, ITQ-53) or phosphazenes (ITQ-47) as OSDAs, which contain P-C and P-N bonds, respectively. [1]

Here, we report the use of a novel family of OSDA, the aminophosphonium cations, with both P-C and P-N bonds in their structures. Particularly, the cation 1,4-butanediylbis[tris(dimethylamino)]-phosphonium was used as OSDA and a new zeolite, named ITQ-52, has been achieved. [2]

Due to the severe peak overlapping, the structure of ITQ-52 could not be determined using laboratory X-ray diffraction data. In fact, even the true unit cell resulted to be elusive, being monoclinic with one angle extremely close to 90°, and then easily confused with an orthorhombic cell. So, all the preliminary attempts for solving the structure as orthorhombic failed.

New X-ray diffraction data were collected at beamline MSPD of the Spanish Synchrotron ALBA. The high resolution achievable using the MAD26 detector allowed determining the small deviation of one of the angles, and then that its true unit cell was monoclinic ($a = 17.511$ Å, $b = 17.907$ Å, $c = 12.367$ Å and $\beta = 90.22°$, space group I12/m1). Subsequently, the complete structure could be solved using the program FOCUS, showing that the unit cell of zeolite ITQ-52 contains 10 independent Si positions and 19 O positions, and presents a bidirectional pore system formed by channels of 8R and 10R that intersect one to each other generating large cavities, accessible through two 10R and four 8R apertures.

The structure found for ITQ-52 is in good agreement with the data obtained from solid state MAS-NMR and N2 and Ar adsorption, among other techniques.

References

[1] M. Moliner, F. Rey, A. Corma, Angewandte Chemie International Edition 2013, 52, 13880-13889

[2] Raquel Simancas, José L. Jordá, Fernando Rey, Avelino Corma, Ángel Cantín, Inma Peral, Catalin Popescu, J. Am. Chem. Soc. 2014, 136, 3342-3345

Caption (s) - Add figures as attached files (2 fig. max)

Figure 1. Rietveld refinement of the X-ray powder diffraction pattern of calcined ITQ-52

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