Structural Characterisation and Properties of New Microporous Materials

João Rocha[a], *Department of Chemistry, CICECO, University of Aveiro, 3810-193 Portugal.* E-mail: rocha@dq.ua.pt

Zeolites are crystalline, hydrated aluminosilicates with open three-dimensional structures built of SiO_4 and AlO_4 *tetrahedra* linked to each other by sharing all the oxygens to form regular intracrystalline cavities and channels of molecular dimensions. These materials possess remarkable physical and chemical properties, such as selective sorption, ion exchange and catalytic activity.

Mixed octahedral-pentahedral-tetrahedral (heteropolyhedra) microporous (OPT) framework silicates are zeolite-type materials synthesised and comprehensively studied since the early 1990s [1]. Examples include silicates of Ti and other metals, such as Zr, Nb, V and Sn and Cu. With the advent of the nanotechnology era, and the increasing interest in the use of molecular sieves for device applications, the constituent elements of OPT materials have been further extended to the lanthanide metals, exploring properties like photoluminescence [2].

OPT materials are often prepared in the form of microcrystalline powders (sometimes with considerable degree of disorder) and, thus, single-crystal X-ray diffraction (XRD) is not generally used. Here, we wish to show how a combination of powder XRD and advanced solid-state NMR (among other) techniques allow the resolution of the crystal structures of these materials. A brief account of some of the materials properties will also be given.

[1] Rocha J., Anderson M. W., *Eur. J. Inorg. Chem.,* 2000, 801. [2] Rocha J., Carlos L. D., *Curr. Opin. Solid State Mater. Sci.,* 2003, **7**, 199.

Keywords: zeolites, structure, lanthanides