175
Structure and Bonding

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Luis Gómez-Hortigüela
Editor

Insights into the Chemistry of Organic Structure-Directing Agents in the Synthesis of Zeolitic Materials

With contributions by

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Preface

Since their first use, the addition of organic species (usually organic cations) to the synthesis gels of zeolite materials has triggered the most important revolution in the preparation and discovery of new zeolitic materials with unprecedented properties. These organic species drive the crystallization pathway toward a particular zeolite framework type with specific chemical properties, and hence they are referred to as organic structure-directing agents. During the crystallization process, these organic agents organize the inorganic units into a particular geometry from which viable nuclei of the host-guest system will be produced, which will promote the crystallization of a certain zeolitic material. The use of organic structure-directing agents has enabled the discovery of a large number of new zeolite topologies, with very different pore shapes and sizes; in addition, they have made accessible particular chemical compositions of zeolite networks. Both of these factors have greatly amplified the number of applications of this important class of materials in different sectors of the chemical industry.

Traditionally, the main properties whereby researchers designed new organic structure-directing agents focused on their size, shape, and hydrophobicity (chapter "Introduction to the Zeolite Structure-Directing Phenomenon by Organic Species: General Aspects"). However, and due to the complexity of the crystallization process of zeolite materials, a deep knowledge of the chemical role played by these organic species was not available. As a consequence, research on the use of organic structure-directing agents was mainly based on a trial-and-error basis, carrying out systematic explorations of the structure-directing ability of different organic species and synthesizing new materials, but basing the research efforts only on empirical evidence and chemical intuition. Nevertheless, one of the major aims in this research field is the rational design of organic structure-directing agents for the synthesis of a targeted zeolite material. This, which was not possible just a few years ago, is starting to become accessible thanks to the great advancement of mainly two physico-chemical techniques that have greatly enhanced our knowledge of the organic structure-directing phenomenon: (1) diffraction techniques (chapter "Location of Organic Structure-Directing Agents in Zeolites Using Diffraction

Techniques"), which now allow to find the location of the organic species within zeolite frameworks, enabling the establishment of structural relationships between zeolite topologies and the geometrical properties of the organic structure-directing agents that drive their crystallization, and (2) molecular modeling techniques (chapter "Molecular Modelling of Structure Direction Phenomena"), which have allowed to understand, from a molecular level, the structure-directing mode of action of these organic species. In addition, and based in part on the knowledge gained through these techniques, in recent years new chemical concepts are emerging in structure-direction of zeolite frameworks by organic species. In this context, the spectrum of organic compounds, which was originally almost exclusively based on quaternary ammonium cations (based on nitrogen), has been notably amplified by the use of alternative organic cations based on phosphonium or sulfonium ions (chapter "Beyond Nitrogen OSDAs"), or by organometallic compounds (chapter "Metal Complexes as Structure-Directing Agents for Zeolites and Related Micro porous Materials"), providing new structure-directing agents with novel chemical properties that can be transferred into zeolite materials. Not only the use of new types of organic compounds but also the appropriate use of intermolecular interactions that trigger a remarkable supramolecular chemistry during the structure-direction phenomenon has provided with new zeolitic materials (chapter "Role of Supramolecular Chemistry During Templating Phenomenon in Zeolite Synthesis"). The geometrical correspondence between organic structure-directing agents and zeolite frameworks has additionally enabled a strategy to tackle one of the greatest challenges in zeolite (and materials) science, the search for enantiopure chiral solids able to perform enantioselective operations (chapter "Chiral Organic Structure-Directing Agents"). All these aspects that will be covered in the different chapters of this book have notably enhanced our knowledge on the organic structure-directing phenomenon during the crystallization of zeolites, and have led to new complex materials with novel and sometimes unprecedented properties that have greatly expanded the range of applications of zeolites in different fields.

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Contents