Elucidating the Structures of Nanoporous Microcrystals

Lynne B. McCusker, *Laboratory of Crystallography, ETH-Hönggerberg, CH-8093 Zürich, Switzerland.* E-mail: lynne.mccusker@mat.ethz.ch

With their stable and open aluminosilicate framework structures, zeolites and their analogs have proven to be ideally suited for intriguingly diverse applications. Their pore openings, which range from 0.25 to 2.0 nm, have molecular diemensions; their void space can reach up to 50% of the total volume; they are crystalline with well-defined and ordered pores; and their framework structures are anionic or neutral. These features are exploited in their use as molecular sieves, as shape-selective catalysts, as dessicants, as ion-exchangers, and as hosts in advanced materials. A zeolite's suitability for a specific application is highly dependent upon its structure, so structure analysis is an intrinsic part of zeolite science. However, because most zeolites can only be prepared in polycrystalline form, standard methods of structure analysis cannot be applied.

Over the years, zeolite crystallographers have devised a number of different methods to overcome or circumvent this problem. Initially, physical model building based on information from various sources was the only option available. Interestingly enough, this is probably still the most powerful tool in the zeolite crystallographers toolbox, but it requires experience, talent and intuition. As computing capacity has increased, however, algorithms for automating the model building process have been created. At the same time, methods for improving the quality of reflection intensities extracted from powder diffraction patterns have been devised, and this in turn has allowed single-crystal methodology to be applied with greater success. An overview of some of the more recent developments in this field will be presented.

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