Zeolites are increasingly important materials in industry, particularly as catalysts. Neutrons are ideal probes of their behaviour

Marvellous zeolites

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Zeolites are used as catalysts in the petroleum industry

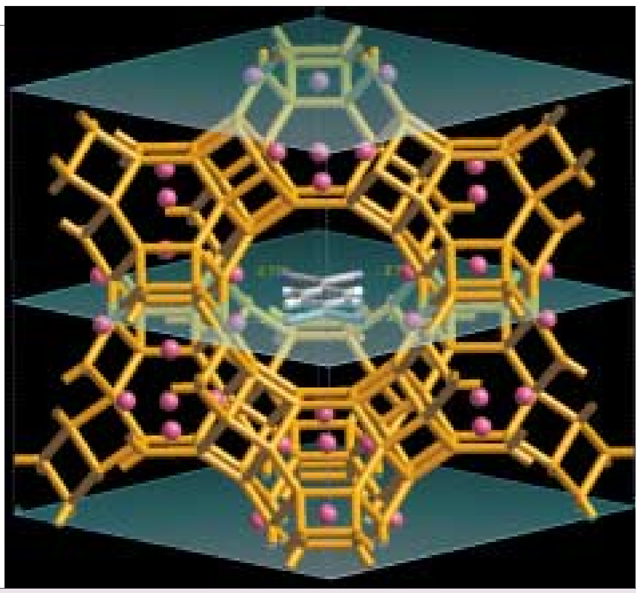
Zeolites are remarkable minerals with a crystal structure consisting of a porous aluminosilicate framework which creates a system of linked channels and cavities. Atoms, ions (charged atoms) and molecules can enter the framework, and this property also makes zeolites extremely useful.

In naturally-occurring zeolites, the cavities are filled with water and possibly lightweight metal ions such as those of sodium, potassium or calcium, which can be exchanged for other ions. One of the first applications of zeolites was as water softeners to remove calcium ions from hard water. The minerals' absorptive and ion-exchange abilities are, in fact, the basis for many washing powders.

Zeolites, however, have many other important uses, particularly in the chemical industry. Zeolites with straight channels less than a nanometre across are widely used as 'molecular sieves' to separate molecules of different sizes and shapes such as similar hydrocarbons but with either a straight-chain or branched structure.

Perhaps the most exciting applications are as catalysts, bringing about specific and selected chemical reactions. They are used in the petroleum industry to break down or 'crack' heavy, oily hydrocarbons into lightweight products like gasoline. Zeolites are considered to be much more environmentally friendly than other traditional catalysts. They are also increasingly being used to make various organic chemicals. Ionic exchange can introduce catalytically active metal ions like those of copper or the rare earths, which are then constrained by the geometry of the zeolite framework to carry out only specific reactions giving compounds in high yields.

The arrangement of 7,7,8,8-tetracyanoquinodimethane in the pores of zeolite NaY



The new synthetics

Natural zeolites are not adequate for that many applications. A large number of synthetic zeolites have therefore emerged on the market, the most common being zeolites X and Y (with the structure of the mineral faujasite) and ZSM-5. A great deal of effort has also gone into fabricating new materials with different pore systems, like the mesoporous MCM-systems developed by the American company Mobil.

Establishing how and where molecules are absorbed in the zeolite structure is the basis for understanding the behaviour of such systems and their applications. Neutrons are particularly suited to studying both the structure and the dynamics of water or organic molecules in the voids and channels of zeolites. We can incorporate different 'probe' molecules and study them. For example, we used neutron diffraction to determine the location of an organic molecule 7,7,8,8-tetracyanoquinodimethane in the supercage of a zeolite Y, shown opposite. You can see how the molecule is attached to the zeolite framework.

The sensitivity of neutrons for hydrogen and other light atoms allowed us to locate the organic molecule. The results of structure determination is supported by molecular dynamics calculations. The dynamics of these 'guest' molecules can be followed by inelastic incoherent scattering, therefore complementing nuclear magnetic resonance experiments, which are on a different time-scale. Neutron scattering thus provides not only basic knowledge but also supports important industrial processes. ■

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