Crystals and chemistry: the zeolites

The science of crystallochemistry was born at the beginning of the 20th century with the discovery of X-rays. Its objective was to explain the relationship between the properties, chemical composition and arrangement of the atoms in crystals.

Electron microscopy view of zeolites

There are a multitude of zeolites. Their impact on everyday life is enormous; they are used in water softeners for domestic appliances, as catalysts in the petrochemical industry and even to trap the odours in cat litter!

The boiling stone: an amazing crystal

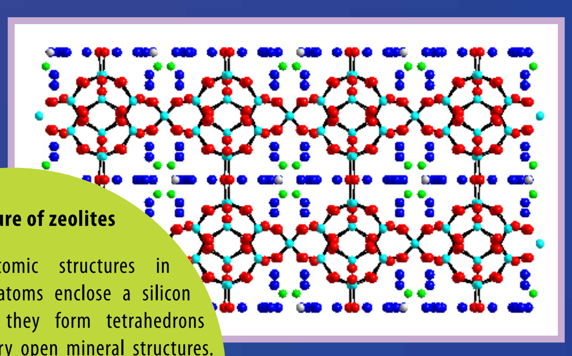
In 1756 Cronstedt made an astonishing discovery: when heating a sample of the mineral stilbite to around 150°C he found that it became covered in bubbles, as if the stone was boiling. The mineral is now known as «**zeolite**», from the Greek *zeo* (to boil) and *lithos* (stone).

X-rays provide evidence of the nano-porous structure of this compact crystal

In 1930 Taylor and Pauling started to use X-ray diffraction to study the first zeolite crystals. They revealed that these minerals are made up of a nano-porous matrix at atomic level. Stilbite is a sodium calcium aluminium silicate which can hydrate or dehydrate in a reversible manner, according to the temperature. Water is trapped within the cavities of the structure.

There are around 50 natural zeolites and more than 500 artificial zeolites in existence

This **crystallographic** approach to atomic arrangement was a real revolution for chemists, who were thus able to visualise the structure and constitution of isolated solids and thus focus on the development of synthetic new materials.



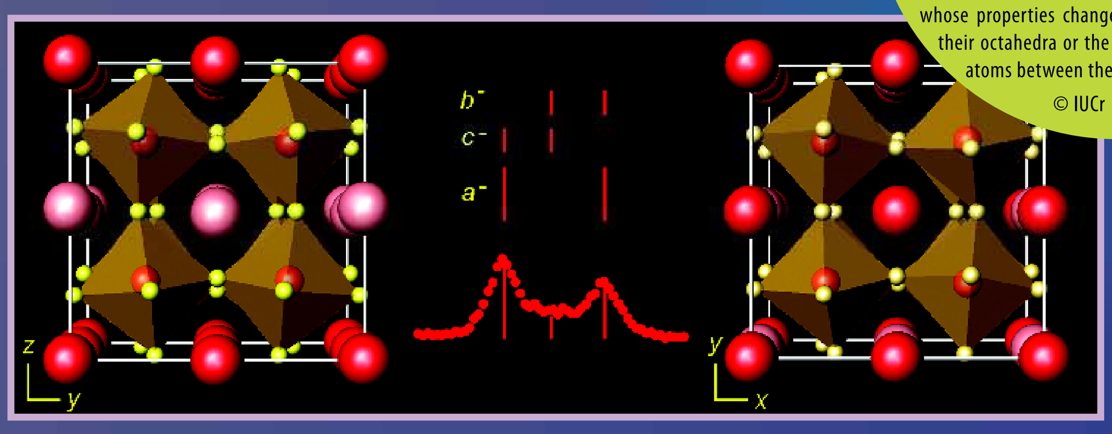
The structure of zeolites

Zeolites have atomic structures in which four oxygen atoms enclose a silicon or aluminium atom; they form tetrahedrons generating rigid and very open mineral structures. The cavities are occupied by cations (such as calcium or sodium) and water molecules. These cations can be extracted from the crystal reversibly by moderate heating and this perfectly explains the mystery of the «boiling stone».

Some typical zeolites:
Chabazite, Melbourne (Australia)
Heulandite, Teigarhorn (Iceland)
Stilbite desmin, Teigarhorn (Iceland)
Coll. Muséum de Grenoble

Crystallography in the design of new materials

Crystallography is essential in solid-state chemistry: the determination of a crystal's structure shows the relationship between its structure at the atomic scale and its properties observed with the naked eye. With advances in crystallography, chemists can «understand» existing materials and, more importantly perhaps, design new materials with the desired properties, by modulating the assembly of atoms. This is the case, for example, in materials with a perovskite structure, whose properties change with the orientation of their octahedra or the chemical nature of the atoms between these octahedra.



X-ray diffraction on crystalline powders can be used to determine the structure of molecules