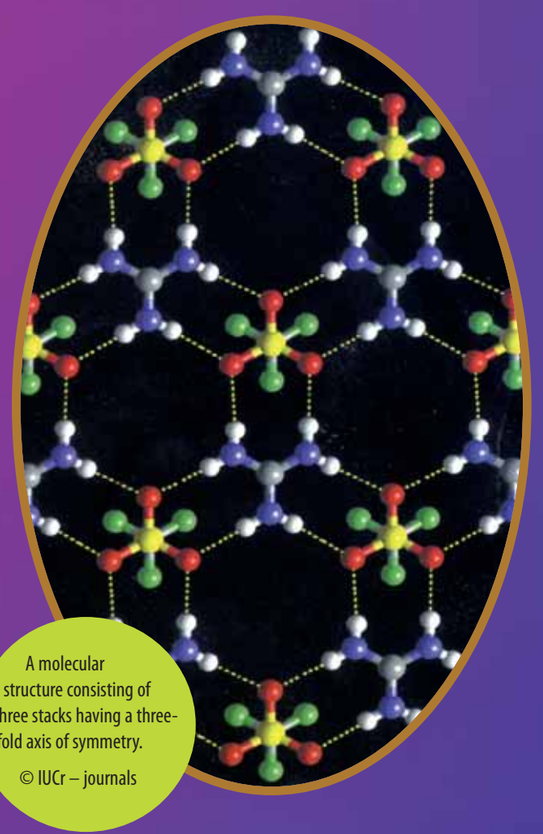
Diffraction of crystals gives a bar code of materials

Crystals are essential to modern society, their study using diffraction of X-rays electrons or neutrons gave birth to crystal chemistry, at the beginning of the 20th century. Crystal chemistry's objective is to explain the relationship between the properties, the chemical composition and the atomic arrangement in materials.



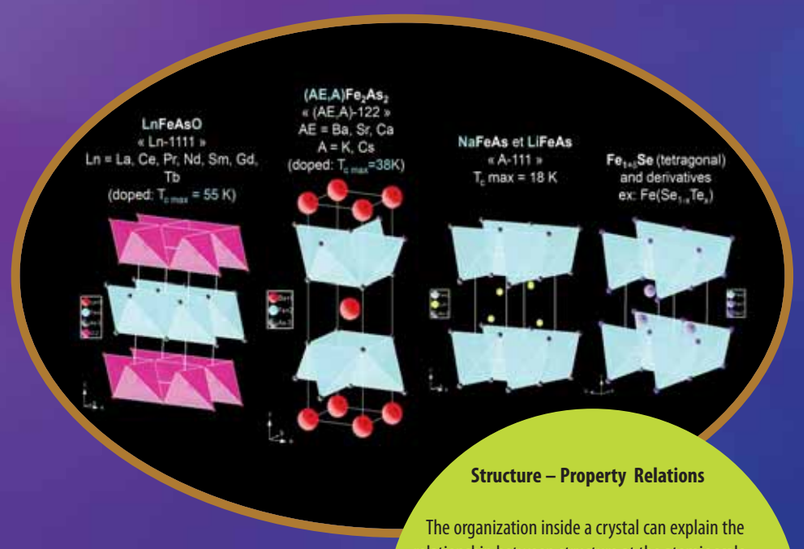
A molecular structure consisting of three stacks having a three-fold axis of symmetry.

The crystallographic approach

The crystallographic approach to understand atomic arrangement represented a revolution for science. For the first time, we could directly see the atomic structure and make-up of materials. This enabled scientists to focus on developing strategies for making materials with new and/or improved physical properties, e.g. new generation batteries, new materials for hydrogen storage... etc.

Applications for crystallography today exist not only in **material science**, but also in the synthesis and structure determination of new molecular materials including the development of **new medicines**.

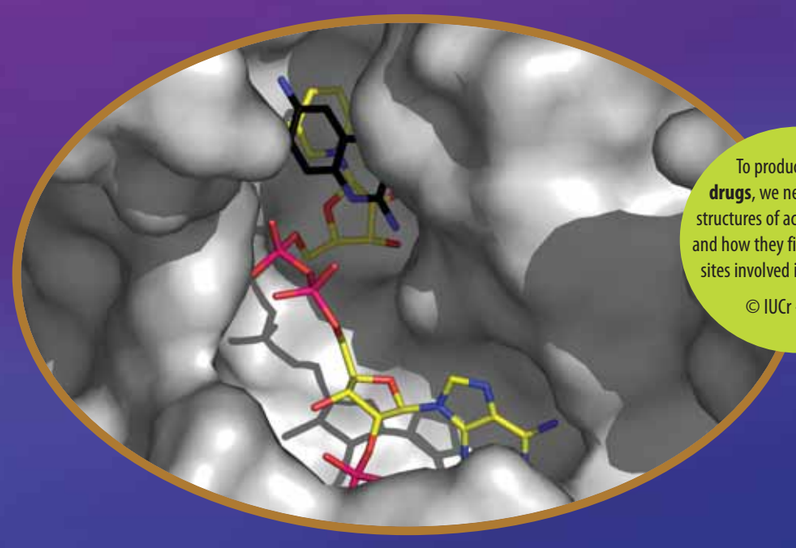
In principle, if a compound or substance can be crystallised, its structure can be determined by X-ray crystallography



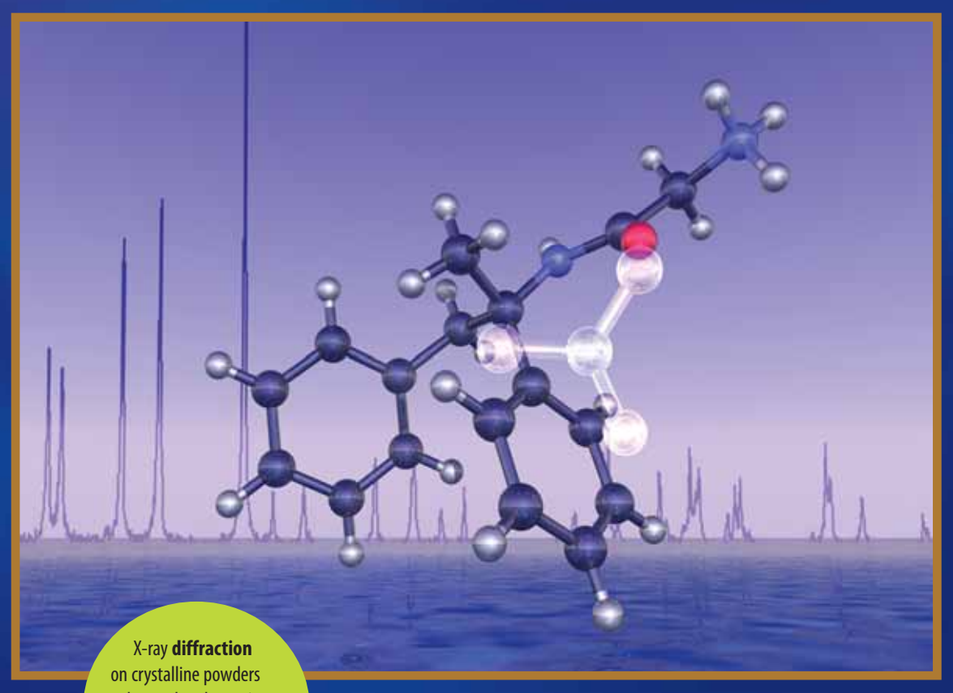
Structure – Property Relations

The organization inside a crystal can explain the relationship between structure at the atomic scale and macroscopic properties. With advances in crystallography, chemists can "understand" existing materials and try to design new materials with desirable properties. This was the case for "copper oxide superconductors", and more recently, iron-based superconductors as well.

source : Institut Néel-CNRS



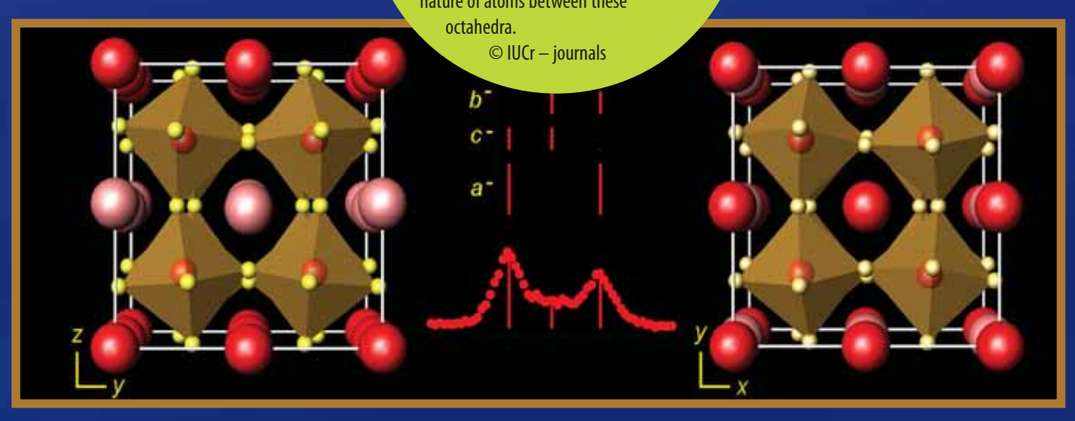
To produce new **drugs**, we need to see the structures of active molecules and how they fit into the target sites involved in their actions.



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

Perovskite, the name of a crystalline structure with many different properties.

They are basic blocks of some superconductors, ferroelectrics and materials in computer hard drive. In such materials there is a relationship between the order on the atomic scale and physical properties. The properties depend on orientations of the octahedra as well as the chemical nature of atoms between these octahedra.



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