A polycrystalline material or ‘powder’ is an ensemble of several randomly oriented crystallites. The size of the elementary crystals is of the order of micrometer. Microcrystalline compounds cannot be singled out to be characterized in the same way as single crystals. Chemical matter, drugs, minerals, heritage manufactures can be available or can be reduced in the form of crystalline powders.

**The study of powder is often a challenging task.**

### X-ray phase identification in a powder mixture: Qualitative Analysis

An X-ray powder diffraction pattern is characterized by a unique distribution of both positions and intensities of Bragg peaks. Each individual crystalline compound has its own “fingerprint”, which enables the utilization of powder diffraction data in crystal phase identification.

A digitized representation of powder data is quite compact and is especially convenient for comparison with other patterns, provided a suitable database is available.

### Crystal Structure Determination by X-ray powder diffraction

X-ray diffraction is undoubtedly the most important and powerful methodology for elucidation of crystal structures, widely adopted in several scientific fields and technological applications: solid-state chemistry, pharmaceutical, materials science, mineralogy, cultural heritage, ...

A detailed description of the molecular structure is fundamental for understanding the structure-property relationships.

**POW_COD database**

Downloads: 1059

Users: 1039

**QUALX2.0 and POW_COD database are software tools developed by IC for phase identification.**

**QUALX2.0 software**

Downloads: 5090

Users: 4639

**EXPO2014 software**

Downloads: 5568

Users: 5734

### OChemDb: Open Chemistry Database

A database dedicated to collect, to make available by statistical tools and to manage crystal chemical information coming from the CIF files contained in the Crystallography Open database (COD). **OChemDb** can be used for searching and analyzing crystal-chemical information (bond distance, bond angle, space group, ...) of structures already solved, to be used for different scientific purposes.