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Structural characterization of crystalline materials (with different complexity) by Single-Crystal Diffraction Analysis

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Single-Crystal X-Ray Diffraction (SCXRD) is a powerful non-destructive analytical technique commonly considered as the main tool for the structural characterization of crystalline materials at the atomic level. For this reason, SCXRD is very useful for a wide range of disciplines such as chemistry, biology, materials science, or pharmacology in both academic and industrial settings.
The structure solution of small molecules is today considered a routine, if not trivial, process, that involves different steps such as crystallization, data collection, initial phasing and structure refinement. This process allows to provides detailed information about the atomic arrangement of crystalline compounds, including bond-lengths, bond-angles, and details of site-ordering. Its contribution is therefore fundamental to understanding the physicochemical properties of many substances and their relationships with the structure in crystalline materials.
In contrast, the crystal structure determination of macromolecules is a complicated, often still challenging, multi-step process, that involves the availability of different types of data (e.g. high resolution XRD data, SAD data, molecular models suitable for MR) and the combination of different tools (e.g. EDM techniques, efficient algorithms for substructure location and/or for phase extension, restrained least-squares procedures).
When single crystals of sufficient dimensions are not available, electron diffraction (ED) may be considered a useful alternative technique; unfortunately, the quality of the crystal structure models obtained by structure refinement is not comparable with that usually obtained by XRD.
IC researchers have a long tradition in the development of innovative crystallographic methods for the structure solution of molecules with different composition and complexity, by XRD as well as ED techniques. The core of these theories is implemented in automatic software (i.e. the SIR family), widely used by the scientific community.
This webinar aims at providing a brief overview of the technique, methods and strategies for a successful structure solution and some applications to real cases.

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