

**MS13-1-13 X-ray Diffraction and Diffusion Measurement Facility of the Institut Jean Barriol
#MS13-1-13**

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Abstract

The PMD²X (Plateforme de Mesures de Diffraction et de Diffusions des Rayons X) of the Institut Jean Barriol (FR 2843) [1-2] offers a first-class diffractometry service, both nationally and internationally. It was evaluated and certified in 2020 by the INFRA⁺ Lorraine University of Excellence quality programme to obtain the status of Structure d'Appui à la Recherche (StAR). Located in Vandoeuvre-lès-Nancy at the CRM2 laboratory (UMR UL-CNRS 7036), on which it relies instrumentally and methodologically, it provides the entire scientific community and industrial partners with analysis and characterization approaches appropriate for different types of functional materials (organic, inorganic, nanomaterials, etc.).

Equipped with a wide range and original devices allowing samples to be placed in non-ambient conditions, it allows:

- Measurements under extreme conditions (temperature, pressure, electric field, laser excitation, controlled humidity, gas flow, etc.)
- Phases identification and quantification from the structural parameters measured by X-ray diffraction
- Studies of phase transitions (coupled with DSC measurements)
- Nanoparticle and crystal domain sizes
- Interatomic bond lengths
- Molecular conformation
- Crystal packing
- High resolution crystallography and electron density modelling
- Energy calculations of inter-molecular interactions and electrostatic properties
- Analysis temperatures from 5 K to 720 K (-268°C to 450°C)

Single crystal studies: PMD²X performs on-demand and in routine, structure resolutions of small molecules. It provides crystallographic and structural information on your compounds (figures, CIF files, interatomic distances and angles)

- Crystal size = 50 to 200 µm (Recrystallisation possible)
- Temperature from 5K to 500K (by nitrogen or helium jet)
- X-ray sources available: Copper, Molybdenum, Silver.
- 4 circle goniometers and CCD detector, Bruker CMOS Photon III.

Powder studies:

- Reflection and transmission measurements.
- X-ray sources available: Copper Kalpha1 and Molybdenum.
- Identification and quantification of crystalline phases
- Monitoring of phase transitions (temperature: 11 K to 720 K)
- Analysis of mesoporous structures
- Characterization of nanomaterials, nanoparticles and confined liquids with the pair distribution function (PDF) method.

- PMD²X develops partnerships with large facilities (Synchrotrons) both through its involvement in the RECIPROCS network but also through new collaborative projects.

- The PMD²X platform is also strongly involved in the promotion of crystallography in Africa through the IUCr-UNESCO Open-Labs and the new Remote-Lab projects. These actions are also associated with hosting and training of young African researchers.

References

- [1] www.crystallography.fr
[2] <http://crm2.univ-lorraine.fr/lab/fr/services/pmd2x/>

Examples of crystallographic analysis possibilities

