LABORATORY OF CHEMICAL CRYSTALLOGRAPHY

Dipartimento di Scienze Chimiche e Geologiche – UniMORE

Centro Interdipartimentale Grandi Strumenti – UniMORE

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CONDITIONS FOR

- **Collaboration on a shared scientific project**.[1] The Laboratory of Chemical Crystallography (LCC) is interested in scientific collaborations entailing X-ray crystallography as a key characterization tool. The involvement of LCC is subject to the following conditions:

  1) LCC accepts only scientific collaborations in which X-ray crystallography is used to solve well-defined scientific problems (e.g. structural studies on new compounds, absolute structure determination, characterization of phase transitions, study of polymorphs, etc.). Please describe your research project (no more than 5000 characters), attaching any relevant publication; justify the use of X-ray crystallography for characterizing your samples; [2]
  2) LCC will take care of all steps in structure analysis including unit-cell measurement, data collection and reduction, structure solution and refinement, absolute structure determination (when relevant), presentation of results according to publication standards and search of crystallographic databases;
  3) upon mutual agreement, LCC will carry out any additional chemical operation that may become necessary (additional re-crystallizations, purifications, etc.);
  4) based on the available resources and manpower, for each established scientific collaboration no more than *two* complete structural analyses *per month* can be carried out; please indicate the number of samples you wish to measure or check; for each sample, please fill in the **sample information sheet** given below;
  5) the crystallographer will **share the coauthorship** of the resulting publication(s).

[1] All collaborations and services will be handled using the strictest confidence and no information gained at any stage will be disclosed to third parties.

[2] LCC will decline collaborations that are not supported by a focussed research project, or in which X-ray crystallography is used to duplicate information already available from other techniques; LCC will not perform a blind screening of otherwise uncharacterized samples; such activities must be run as X-ray diffraction services.

- **X-ray diffraction service**.[1] LCC offers a complete, cost-effective crystallographic service for structure determination on single crystals of organic, inorganic or metal-organic compounds excluding macromolecular species. We routinely handle air-sensitive materials (due to oxidation or solvent loss) and disordered or twinned samples, which require special efforts in data collection and structure refinement. We also carry out additional operations and studies in chemical crystallography, as detailed below. The crystallographer will not share the coauthorship of the resulting publications, but the contribution of LCC needs to be acknowledged. For each sample you wish to measure or check, please fill in the **service request form** and the **sample information sheet** given below.

  Available services and costs are:

  - (*only as a prerequisite for subsequent work*) search of crystallographic databases (**0 €**);
  - (*only for organic compounds and as a prerequisite for subsequent work*) sample recrystallization by thermal, liquid-diffusion or vapour-diffusion methods (**50 €** *per* sample);
  - unit-cell measurement (**50 €** *per* crystal or **100 €** for statistics over 3 crystals from the same batch);
  - complete structure determination (unit-cell measurement, data collection, structure solution and refinement, determination of absolute structure when relevant) with data delivery in *cif* format (**500 €** *per* structure);[3,4]
  - analysis of structural parameters (interatomic distances, interbond angles, torsion angles, conformations, crystal packing, hydrogen-bond interactions, etc.) and preparation of high-quality publication data (tables and graphics) (**200 €** *per* structure);
  - face indexing of as-received single crystals for subsequent physical studies (**100 €** *per* crystal);
  - homogeneity check on bulk microcrystalline samples by X-ray powder diffraction through comparison with single-crystal data (**100 €** *per* sample);
  - elemental analysis on C, H, N, S (**50 €** *per* sample);
  - ^{1}H NMR for the individuation and quantification of disordered lattice solvent (**50 €** *per* sample).

[3] The reported costs will be applied only for successful structure determinations with delivery of publication-quality results, irrespective of the amount of work required; if the data collection yields unpublishable structural data, or in the event that the crystallographer decides not to proceed with data collection due to insufficient crystal quality or size, only unit cell measurement will be charged.

[4] No extra costs will be charged in case special procedures are needed to obtain the highest-quality data from air-sensitive or very soft materials (e.g. low-temperature data collection, mounting of the crystal in a glass capillary, etc.); unless otherwise requested, the crystallographer will choose the most convenient setting for the experiment.

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Name: Position:

Department/Institution: Address:

SERVICE REQUEST FORM

Sample number/code: _____

(*tick as appropriate*)

- ○ (*only as a prerequisite for subsequent work*) search of crystallographic databases;
- ○ (*only for organic compounds and as a prerequisite for subsequent work*) sample recrystallization by thermal, liquid-diffusion or vapour-diffusion methods;
- ○ unit-cell measurement on _____[5] crystals;
- ○ complete structure determination (unit-cell measurement, data collection, structure solution and refinement, determination of absolute structure when relevant) with data delivery in *cif* format;
- ○ analysis of structural parameters (interatomic distances, interbond angles, torsion angles, conformations, crystal packing, hydrogen-bond interactions, etc.) and preparation of high-quality publication data (tables and graphics);
- ○ face indexing of _____[5] as-received single crystals for subsequent physical studies;
- ○ homogeneity check on bulk microcrystalline samples by X-ray powder diffraction through comparison with single-crystal data;
- ○ elemental analysis on C, H, N, S;
- ○ ^{1}H NMR for the individuation and quantification of disordered lattice solvent.

Determination of absolute structure is:

○ required ○ not required

Other details on sample handling and measurement conditions:

[5] Indicate the number of crystals to be measured.

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Name: Position:

Department/Institution: Address:

SAMPLE INFORMATION SHEET

Sample number/code: _____

The sample comprises:

(*please tick one or more items as appropriate*)

- ○ selected single-crystals
- ○ mixture of powders and single-crystals to be selected by the crystallographer
- ○ solid phase(s) only
- ○ solid phase(s) plus mother solution or maintenance liquid
- ○ (presumably) air-stable material
- ○ (presumably) air-sensitive material due to solvent loss or oxidation
- ○ only light atoms (second-row elements + H)
- ○ one or more heavy atoms

The chemical nature of the sample is:

(*provide all available information, including tentative formula, expected structure, crystallization conditions like technique, solvent, temperature, etc.*)