

# X-RAY SAMPLE SUBMISSION

## Single Crystal Sample Information

All samples submitted to the X-ray Facility for characterization must be accompanied by a [Submission Form](#). Samples must be clearly labeled and stored under mother liquor if they are sensitive to solvent loss. Air-sensitive samples should be tagged as such. Any special handling instructions should be clearly noted on the submission form. Since crystal quality is probably the single most important factor in determining the final precision for a given structural investigation, keep in mind that high-precision structural results will generally require high-quality crystals.

In general, crystals should meet the following criteria:

1. The crystal should be a single entity which has no smaller crystals or powder attached to it.
2. Crystals should be of the proper size and shape. The crystal should be 0.1 to 0.6 mm. on an edge and as equidimensional as possible. For substances which do not contain highly absorbing elements (e.g. most organic molecules), the optimum sample would be a ~0.5mm. diameter sphere. Needle- or plate-shaped crystals can usually be used if they are at least 0.1mm. thick.
3. Good single crystals usually have well-defined and lustrous faces; they are of uniform color and contain no cracks or fracture lines.
4. Crystals should diffract to reasonably high scattering angles
5. Crystals should have reasonably uniform and small “mosaic spreads”.

## Procedure for “Hands-On” Use of Facility Instruments

1. Contact lab manager for access to training documents and training website. (See [X-ray Lab Manager](#)).
2. Complete training course on the use of the machines and x-ray safety.
3. Fill out the [Submission Form](#) for single crystal and powder samples.
4. For single crystal samples, see the [X-ray Lab Manager](#) to reserve time on the x-ray diffractometer and obtain a WFU X-ray Code Number. Record the code on the sample submission sheet. All data files will be stored under this code and structures will be referenced by this code. User priority is determined by the [X-ray Lab Manager](#)
5. For powder and/or thin film samples, reserve time on the D2PHASER or D8DISCOVER using the on-line calendar. Contact the [X-ray Lab Manager](#) to get access. Note: when using the D8DISCOVER, all experiments that involve a change in instrument configuration must be coordinated through the [X-ray Lab Manager](#).