Experimental Report
ID: MA5143

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The setup for measurements was ready at the beginning of our session. In order to get the instrumental parameters of the system to use into CrysAlisPro software we measured a YAG sample (Y3Al5O12 Space group: Ia3d) at RT conditions.

A total of 15 MOF's samples were measured at 100K in three different Chi positions (-45, -25 and 0º) with a fully Phi rotations with a step of 0.25º doing a total of 1440 images for each measurement.

Our samples were very sensitives in air and in general, for each sample, we had to try several crystals in order to get good diffraction images. Unfortunately, our crystals were a bit small (5-10 µm size) and their power diffraction was also very small obtaining only a diffraction peaks to low resolutions (around 1.5Å or less).

The version of CrysalisPro proposed to work for the beamline staff was a very old version and we decided to check the last version available on the Rigaku site (42.53a). Following the indications given in the beamline, each dataset can be worked independently but not together. Currently, we are working with the software team of Rigaku in order to resolve this problem. In this way, we hope to also be able to help for future users of this beamline.

Currently we are working on the datasets measured and try to resolve and refinement of the structures for the different compounds.

Suggestions

1.- The use of a magnetic base in the goniometer head would facilitate the exchange of sample without having to move the goniometer head on the diffractometer. Mainly if you need to check the quality of sensitive crystals.

2.- The information on the head of the CBF files are not correct. Some procedure should be implemented that does it automatically according to the current parameters of the setup used.

Javier González-Platas

IP of the present proposal