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Minutes Of The 1st Spanish Users Meeting Of The XALOC-BL13 Beamline At Alba

ABSTRACT

Minutes of the 1st Users Meeting of the XALOC-BL13 Beamline of Alba. This document describes and summarizes some of the issues that were discussed in this meeting.

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Distribution list		

1 Attendees

On October 22, 2007, the 1st Users Meeting of the ALBA XALOC-BL13 Beamline was held in the Sala de Juntes of the UAB (Bellaterra, Barcelona, Spain).

The participants of the meeting were:

Mark J. van Raaij (MJR, USC)

Xavi Carpena i Vilella (XCV, IBMB, CSIC)

Joan Pous (JP, PCB, UB)

Lourdes Campos (LC, UPC)

Inés Muñoz (IM, CNIO)

Pablo Fuentes-Prior (PFP, ICCC, CSIC)

Miquel Coll (MC, IBMB, CSIC)

Maria Solà (MS, IBMB, CSIC)

Silvia Russi (SR, IBMB, CSIC)

Roeland Boer (RB, IBMB, CSIC)

Raquel Arribas (RA, IBMB, CSIC)

Alícia Guasch (AG, PCB, UB)

José Casasnovas (JC, CNB)

Lucy Malinina (LM, CICBIOGUNE)

Núria Verdaguer (NV, IBMB, CSIC)

Fernando Gil Ortiz (FG, IBV, CSIC)

Clara Marco Marin (CM, IBV, CSIC)

Gavin Fox (GF, BM16-LLS)

Juan Hermoso (JH, IQFR, CSIC)

Francisco J. Fernández (FJF, IBMB, CSIC)

M. Cristina Vega (MCV, IBMB, CSIC)

Eva Boter (EB, Alba)

Claude Ruget (CR, Alba)

Salvador Ferrer (SF, Alba)

Wilfried Schildkamp (WS, Alba)

Jordi Juanhuix (JJ, Alba)

Jordi Benach (JB, Alba)

2 Presentations

SF talked about general issues concerning Alba: overall structure, beamlines, time schedule, budget (20 mins). WS talks about BM16, new detector, new motor control. He mentioned that it would be nice to have a beamline dedicated to crystal screening for the phase II. JJ spoke about the optics (20 mins) and JB about the end station of Xaloc (20mins).

3 Optics-related questions

No one seems to have used high-energy x rays in order to minimize radiation damage.

Overall, the percentage of experiments that require changing the energy of the x-ray beam seems to be around 50-60%. Some users hinted even higher numbers though.

They prefer the focused mode (more than 90% of the experimenters) to the unfocused one. Some think that the choice between the focused/unfocused mode depends (other users) 50-50 on user/usage.

The beamline should be able to get as close as possible to the sulfur edge (MJR). This is not so critical due to absorption effects (GF).

Small crystals of about 10-20 μm are most common. It is important to work with small-sized beams and to be able to irradiate different parts of the crystals to collect a complete dataset.

The foreseen detector and diffractometer should allow the user to collect data higher than 1 Å resolution (JJ).

4 Experimental hutch & detector

No one seems to have tried helium cryo-stream for temperatures below 100K. It also appears that most groups have abandoned the helium cryo-stream.

4.1 Diffractometer

The users prefer a horizontal spindle axis, with the spindle/sample pointing towards the user for easy access (JC). They all also recommend having the kappa-rotation available in the diffractometer in order to optimize data collection. The users commented that having the kappa rotation is always good and that they use the mini-kappa approx. 20% of their time. The positioning of the collimator has proven to be a nuisance for some beamlines.

The availability of the kappa-rotation is very useful to reduce crystal damage by using the optimal (minimal) phi scan, it is also very important for crystal positioning according to unit cell/crystal morphology in order to collect good enough datasets (FJF).

The beamstop has to be able to be translated along the beam axis, its positioning perpendicular to the beam is also very important (MC).

MS suggests that we must be able to manually mount the crystals on the diffractometer.

4.2 Viewing system

The crystal sample should be viewed with a large high resolution screen, the sample should be back lit, and one should be able to use an on-axis viewing system. Two cameras may not be a bad idea.

They like very much the viewing/centering system in ID23-2.

The automated centering system in C3D works best with back-lit sample (GF). UV-light may be useful for the centering the sample too.

We should be able to mount capillaries for screening and/or collecting data (GF).

4.3 Additional equipment in the experimental hutch

The A-frame system to hold the detector would be useful (MC), however its stability does not seem to be better than granite blocks, price is the same, space issue since the A-frame takes more space (JJ).

The end station would benefit from a humidity control unit to modify crystallization conditions like the PROTEROS system also called a free-mounting system (FMS). We

should leave available free space in the experimental station for a possible FMS (MC). There is a second FMS in development that may be better than the existing one (MC). PROTEROS is 10% effective in Oxford, UK (MC) which would be great for many projects (MC, JJ). It was cumbersome to use and not so useful at Columbia University (JB).

An optical microscope close to the omega axis for manual handling and mounting of the crystals is compulsory in the experimental hutch.

The users would definitely use a remotely-controlled cryo-shutter.

4.4 Detector

A CCD detector with a hole in the middle (JP) may not be a great idea due to the air-scattering and increased noise (JJ).

No experience with pixel detector(s), so far. CCDs are good enough, they do not care as long as the detector readout is fast.

Users are requested for feedback after going to beamlines having the pixel detector (as per today, only SLS has a pixel detector) (JJ). IM and NV have allocated time there in next months, and they will provide information.

5 Automatization

The automated sample changer should not be too bulky (RA), the resting position or the robot's arm is very helpful (WS). The robot is useful, but it has to be manually removable (MS).

Phi-axis rotation of the gripper/actuator of the robot for screening would be a plus. One starts to see it in other labs (MC) (Oxford diffraction).

Crystallization plate x-ray screening does not seem to be so useful to JC. However, the rest of users seem to agree that plate screening would be extremely useful. Crystallization plate screening can also be useful for crystal screening and even data collection (GF). It seems like the type of plates are the same as the commonly used for crystallization.

ESRF type baskets that are compatible with SPINE-standard pins are the preferred ones, for simplicity reasons and to keep the number of different baskets to be used during synchrotron trips in the laboratory to a minimum.

Some users asked about remote control of the data collection and/or beamline. That'd be nice. Why not program the machine to send SMSs to phone in case of problems? (JB)

5.1 Sample capacity of the robot

More than 50 samples, preferably 200 samples (JC).

The robot that comes with the MD2, the SC3 does not have too much capacity. JC does not like that, because it takes time to replace the baskets (around 20-30 mins, JC) for different users in one shift resulting in poor time usage.

5.2 Speed of the robot

If the robot is too slow, forget about it (JC). It has to be as fast as possible (JC). They agreed that the one in Stanford is too slow. Other users do not show such interest in speed.

6 Auxiliary equipment and computational needs

6.1 Auxiliary equipment

The users seemed to agree that the preparation laboratory should be equipped with a 20 °C incubator and a 4 °C fridge for storage or even growing crystals (IM). They did not comment on the size of them though. General-use pipettes, a simple scale, hood (JB).

They recommend removing the ~~second~~ meeting room (left hand side of the hutches layout) and adding the extra space to the preparation laboratory. This lab should have at least 2-3 microscopes, spare parts: like baskets for the robot, and 2-3 benches.

Laboratory space is more important than office space.

6.2 Sample-amount volume

They seem to converge on an average of 110GB of data collection per day (JS).

These are the (estimated) average days of synchrotron visits per month:

Barcelona/Valencia: 3-6 days 300 crystals a month (10 month/year) (MCV)

Madrid: 2 days 300 crystals a month

Santiago de Compostela: 0.5 days

Bilbao: 1-2 days

Granada: 1 day

Salamanca: 0.5 day

Oviedo: 0.5 day

Zaragoza: 0.5 day

Total: 9-13 days/month

On site: they screen/collect 50 crystals in 6 hours (JC, MCV)

6.3 Backup and computational needs

A real-time backup system would be a plus: that is, a system that backs up the data at the same time it is being collected (FJF).

They prefer high capacity blue-ray DVD's, either automatic (ca. 4000 euros) or semi-automatic to ftp'ing the data after the collection runs. Hard drives are also commonly used for data backups.

Data should be stored from three weeks to one month and six month archive.

Computer speed during data analysis is extremely important but there has to be a compromise between the backup system and the processor speed.

6.4 Software

HKL2000 license by HKL is usually 5% of the purchase cost of the detector per year (JJ) (something like 50,000 euros per year for HKL2000). Users were not aware of that.

In order to fix this problem they can use their own laboratory's HKL2000 license, either when returning to their laboratories with the diffraction frames or by bringing a laptop to the site.

They commonly use XDS, MOSFLM for data integration/scaling and SHELX, SHARP for phase determination. The CCP4 suite has to be available. They recommend having the program STRATEGY in the beamline control computer (RB), JJ and JB disagree with that since it could be harmful during data collection.

7 Possible collaborations

Spectrophotometer: Raman spectroscopy, reactivity (XC).

PROTEROS?

Ask for 6-7 PhD positions to the Ministry of Education.

8 Other

Two full-time beamline scientists may not be enough to run the beamline and/or take care of the visiting users. The users are concerned about the “local contact” figure on site (JH).

FedEx/Mail-in crystallography will eventually become a reality here in Europe. It will not be implemented in day one in XALOC (JJ).

They hope we will offer fast beam time (may be a whole day or one 8-hour shift), as well as long-term projects that will reduce the amount of paperwork to get beam time.