

Powder Diffraction Service of the School of Chemistry
under restrictions of social distancing due to COVID-19 pandemic

The rules have been amended on 15th September 2020

STOE diffractometers George & Ringo

Online booking will be open for both George and Ringo. Please make sure that the measurement programme(s) terminates strictly within the booked slot. If an overnight run is required, please book it together with the preceding 1.5 hour slot and start such run at 16.30.

Following the above instructions ensures that maximum two STOE users will be in the PXRD room **only during the following times: 9.00—9.30; 10.30 – 11.00; 12.00 – 12.30; 13.30 – 14.00; 15.00 – 15.30; 16.30 – 17.00**, which are linked to the established slots in the online booking system Please do not enter the room outside these times.

PANalytical diffractometers John & Paul

Samples for both diffractometers must be submitted **strictly before 12.30 pm on the day of the booked runs.** Please collect the returned samples promptly. Please try to avoid entering the room during the listed above time slots when users of STOE's are likely to be in the room.

SiSub5 holder with zero-background Si inset will be kept in the dedicated and correspondingly labelled of the box with sample holders.

PANalytical diffractometers Pete

Operates as usual: prepare the required paperwork, get it checked and signed by Dr Paul Connor, contact Yuri to arrange the measurement.

Booking Rulesⁱ

MINIFLEX 600

Operated by trained users ONLY, currently:

– Stefan Saxin

The rules for the MiniFlex are:

- Max 2 runs / person and day.
- Samples must not exceed the height of the metal edge on the sample holder.
- All sample holders must be cleaned and returned promptly.

Training will be provided by Stefan Saxin (as of 21st February 2022) to enable more trained users to run their own samples, and as a consequence the service will be diminished over time.

MiniFlex Service

Samples can be submitted twice a day at **10am** and **2pm** Monday–Friday, first come first served.

Booking and submission of samples is done in the same place: on the table outside 223 D.

The MiniFlex service starts Monday 21st February 2022.

Please contact Stefan Saxin (ss948) if you are interested in using the MiniFlex XRD for your own work, e.g. on a regular / semi-regular basis.

PETE

Operated by authorised personnel ONLY.

Please download and read “Outline for Sample Submission”; download, fill and send the “Request Form” using relevant links

from the “Booking” section of the PXRD website.

GEORGE & RINGO

Operated by trained users ONLY.

Training is provided by:

Yuri Andreev

Six 1.5 hour and one overnight run on each of the diffractometers per day.

Each user can book only ONE overnight run PER WEEK on EACH of the diffractometers. Not more than TWO 1.5 hr runs PER USER PER DAY on EACH of the diffractometers.

Booking is compulsory!

Bookable week starts at 9 am each Monday. Online booking for the whole of the current week opens at midnight on Monday. Booked runs can be cancelled, also online and by the person who booked them, not later than 1.5 hours before the scheduled start.

PXRD Administrators reserve the right of cancelling any bookings.

IMPORTANT:

If you cannot collect your capillary on completion of the data collection, but would like to keep it, please leave an empty vial, **with a clearly written your user name** on the latter, on the desk next to the machine and collect it by 5 pm on Friday of the same week, at the latest.

If you find a capillary left on the diffractometer by the previous user, who hasn't left identifiable (see the previous paragraph) vial, please dispose the capillary into the yellow/red plastic bin for sharp glass objects, which is located on the window sill on George side. **Do not leave the capillary within the diffractometer enclosure or on the desk. Do not place the capillary into a vial without clearly written user name on it.**

All vials with capillaries left on the desks will be binned at 5pm on Friday.

The rules in this section are strictly enforced, because improper handling of capillaries and glass vials led to several accidents in the past.

JOHN & PAUL

Operated by authorised personnel ONLY.

Only sample holders provided by the PXRD Administrators can be used on both diffractometers. The most commonly used holders are stored in a plastic pigeon-hole box in the PXRD room decorated by group leaders' initials. Each holder has an engraved ID mark, consisting of the group leader's initials and a number. **You MUST use only holders with the initials of your group leader. Diffraction data from samples placed into non-designated to your group holders will not be collected.**ⁱⁱ

In addition to the most common holders, there is a small number of holders which can accommodate zero-background Si-single-crystal insets (for smaller amount of sample) and are suited for use with Kapton film (to protect from the ambient water or gases). These holders are placed in the pigeon hole marked "Si Sub Air Sens". Kapton film can be obtained from Yuri Andreev.

USE OF UNATHORISED HOLDERS MAY CAUSE SERIOUS DAMAGE AND IS STRICTLY PROHIBITED!

Booking is made online. Starting from midnight, you can book runs on either machine for tomorrow (while still being able to book for the current day until 10 am). Starting from midnight on Friday you can book for the following Monday. Runs can be cancelled, by the person who booked them, no later than 11 am on the day they are booked for.

Prior to booking make sure that the holder you are going to select from the drop list is available on the day of the run!

Each user can book no more than 2 runs/per diffractometer/per day

Only 1 hour and 2 hour programmes for individual samples will be available to users. Please think before booking 2 hour runs. Every longer programme potentially deprives another user from collecting diffraction data on the day!

In the event when you want to collect diffraction data for longer time, please contact Yuri Andreev and provide a justification for such request (pattern collected on the same instrument for 1 or 2 hours; brief description of how the data will be used). Only justified requests will be satisfied, with data collected over weekend.

Samples for Paul must be placed in the dedicated, clearly marked, tray in the X-ray room before 11.30 am on the day of the run.

Samples for John must be placed in the dedicated, clearly marked, tray in the X-ray room before 12.00(noon) on the day of the run.

Measured samples from both machines will be unloaded onto corresponding dedicated trays every morning (except Saturday and Sunday) and MUST BE COLLECTED, EMPTIED, CLEANED and PLACED BACK INTO THE CORRESPONDING PIGEON HOLE WITHIN 24 HOURS for other members of the research group to use.ⁱⁱⁱ **NON - COLLECTED HOLDERS WILL BE MOVED INTO A BUCKET MARKED "Non-collected sample holders from John & Paul" located under the desk with the sample trays.**

PXRD Administrators reserve the right of cancelling any bookings.

ⁱ Complaints about the Rules are accepted only from the Group Leaders

ⁱⁱ There is sufficient number of sample holders to satisfy the PXR D needs of each group. Making sure that all of them are available for use is the sole responsibility of the groups.

ⁱⁱⁱ If such good practice is followed, and enforced, by all members of each research group (and not just by PXR D Administrators) there will always be sufficient number of readily available holders at the time of booking and no need for tracing previous bookings. Let us make this happen!