Procedures for Calculating and Recording Operator Rate Billings

In January 2014, the X-ray Facility adopted a new rate schedule. There are several new charges of which you will need to be aware. The first is a “sample initiation” fee for non-viable samples which are placed on the diffractometer. The second is a charge for unit cell determinations. In addition, one of the biggest changes which affect Authorized Diffractometer Operators (aka “operators”) is the implementation of a variable rate for data collections performed by non-Facility operators. The operator is responsible for calculating and recording these charges for their datasets using software provided by the Facility. **If the operator does not calculate and record the billing properly, the charge for the dataset will be made as if a Facility staff member collected the data. This is a $100.00 charge.** This document outlines the procedure for these new charges and making these variable rate calculations.

Static Charges

The charges which do not depend on instrument time are the **Sample Initiation** fee and the **Unit Cell Determination** fee. This section describes how operators should apply or not apply these charges.

- **Sample Initiation** This charge is made only if an operator places a sample on one of the single crystal diffractometers, and the sample either doesn't diffract, diffracts too weakly, or gives no sensible indexing. Samples which are deemed unsuitable via optical microscopic examination are NOT charged this fee. If the sample is viable and intensity data can be collected or if a reasonable set of unit cell parameters is obtained, this fee is NOT charged.

- **Unit Cell Determination** The charge for a unit cell parameter determination is made under the following circumstances: (a) when the request for single crystal service was for a unit cell parameter determination, (b) the original service request is for either data collection or structure determination, but the quality of the sample is such that sensible preliminary unit cell parameters were obtained, but the diffracted intensities are such that the sample does not merit a collecting a set of intensity data.

Variable Charges

For operator run data collections, the amount of charge for a dataset will depend on instrument time used. The Facility Manager has written a small program which will calculate the rate for you, and its usage is simple. The software's name is `instrument_time.py` and is located in `/usr/local/bin/`.

To receive a short help message, just type on a terminal command line:

```
instrument_time.py --help
```

This will produce the following message:

```
bruker:/~% instrument_time.py --help
Usage: prog [options]

Options:
  --version show program's version number and exit
  -h, --help show this help message and exit
  -N, --nonius to specify the Nonius KappaCCD diffractometer
```
Under normal circumstances, you will only ever use either the -B or the -N options. The -a and -b options are for the Manager’s software testing use only. The procedures for both the Bruker and the Nonius are outlined below.

**Billing on the Nonius**

After data collection has finished, **but before you convert the data to Bruker format**, open a terminal window and go to the directory where the .kcd files have been written. Normally, these files are located in:

```
/home/ccd/kccd_data/<your_advisor's_name>/<structure_ID_code>/
```

When you are in that directory, run this command from the command line:

```
instrument_time.py -N
```

Here is a complete example, assuming the your advisor is Paul Ragogna and the structure ID code is n14015. After logging in and opening a terminal:

```
cd kccd_data/ragogna/n14015
instrument_time.py -N
```

The program will output the following:

Calculating charge for data collected on the Nonius ....
Total hours: 8.00  Total Charge: 49.47

Open up the web page for this sample for editing on the on-line queue and record the amount **49.47** in the Charges text entry box.

**Billing on the Bruker**

After data collection has finished, open a terminal window and go to the directory where the .sfrm files have been written. This is normally

```
/smb/frames/bragg/<your_advisor's_name>/<structure_ID_code>/
```

You can save yourself some typing and get to this directory by using the ~/apex_ccd_data/ symbolic link from the bruker user home directory.

When you are in that directory, run this command from the command line:

```
instrument_time.py -B
```

Here is a complete example, assuming the your advisor is Richard Puddephatt and the structure ID code is b14117. After logging in and opening a terminal:

```
cd apex_ccd_data/puddephatt/b14117
instrument_time.py -B
```
The program will output the following:
Calculating charge for data collected on the Bruker....
Total hours: 16.00     Total Charge: 66.82

Open up the web page for this sample for editing on the on-line queue and record the amount 66.82 in the Charges text entry box.

Please review the X-ray Facility policies located at http://xray.chem.uwo.ca/Rates_Policies.html.