

# Confirming The Sample Orientation

*Alfred Baron, 2023*

Sometimes it is interesting confirm the orientation of a sample after an experiment. This can be done by comparing the positions of the motors in the scan file with those expected from the diffraction code (usually SIXCIRCLE). In general, people are strongly urged to manually print-out the spectrometer angles (“pwh” in specs) and HKL positions (pca6 in either fourc or SIXCIRCLE) and tape these into the log book for every arm position. Then carefully compare them. (It is surprising how often someone accidentally moves to a wrong position). But sometimes users do not make the printouts.

If you want to confirm positions without such a printout then please open the specs scanfile (located in the df/ directory, typically named something like specs\_YYMmmDD where YY, Mmm and DD are the day, month, and year, respectively) using PYMCA\* Load the spec scanfile by selecting file, open and setting the type to all files, then navigate to the specs\_YYMmmDD file and select it. Then (mac) ctrl-click on the scan of interest and select “show scan header” and then select “motors”. Then compare these against the values you expect.

(If you are directly looking the spec scanfile, without pymca, then you should look for the #O lines for the motor names and the #P lines for their positions)

If needed, you can enter the angles from the specs\_YYMmmDD file into the diffraction code and then re-calculate the HKL values (mv(tth=...) followed by “wh6()”) and that will tell you the expected HKL values. Of course, to do that you must first put in the orientation matrix (lattice structure, primary and secondary reflections) as it was determined during the experiment. (If you have printouts from ca6 then the relevant orientation matrix information is included at the top)

Note: at present the interface between the **process\_ixs** code that does batch processing of the spectra in the list file does not save the individual input files for each arm position, including the lists of Q positions. This is expected to be changed in the near future (probably summer of 2023),

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\* PYMCA may be downloaded at <https://sourceforge.net/projects/pymca/> .