Orion

Orion has a closed Eulerian cradle, and especially triple-axis users are normally more familiar to crossed goniometer setups. As a consequence, we want to make you familiar with **using the phi-angle instead.**

For further help, you also may consult:
https://zebra.intranet.psi.ch

Mounting the crystal

It is important, that the crystal is in the geometrical center of the cradle, otherwise all the following procedures are not reliable. A TV camera is installed and aligned for this purpose. If the crystal is perfectly aligned in heigt, x and y, he always will stay in the center of the cross on the monitor, independently of any chi , phi or omega rotation. The chi=90 position is most sensible to a correct height (z), whereas the chi=0 position is sensible to deviations from the correct xy centring (when rotated around phi).

Using Chi and Phi of the Eulerian cradle instead of two crossed goniometers tables:

Phi allows you to turn the sample by 360° around its support axis. This allows compensating for only having one tilt (called chi on ORION) instead of the two goniometer tilts you normally have on a triple axis. By turning phi by 90°, you get access to the "second" (virtual) goniometer table not existing physically at ORION.

Vertical detector window:

The detector has a vertical opening of approximately 28mm at a distance of 320mm (if not changed). This gives access to 5°. If you want to see the next vertical "window", you can move up chi accordingly. We suggest setting this step to (around 3°) to be safe and not to miss the peak.

Searching the peaks:

- *Position the reflection (tau-vector) approximately to a bisecting position (omega=stt/2) enter the cell a b c alpha beta gamma* and *use calctt h k l*
- *Select a chi value to position tau approximately horizontally (if known).*
- *Make an omega scan with steps around 0.1 to 0.25 degrees depending on your mosaic, covering a range sufficiently large (5-15 degrees depending on your initial information).*
- *Select the next chi value*
- *If you found and centered the omega of the peak:*
  make a chi scan with a step of approximately 0.4°
- *now you can normally calculate the turn in phi for the next reflection*

- *you have no idea on the orientation:*
  1) *calculate the stt of a few strong reflections*
  2) *make full ph-scans at various chi positions, approximately 4 degrees apart from each other with fully open detector slits, ph step around .2 degrees by using a command file (example search.go in the directory /home/orionlns/examples)*

Finding the UB:

The UB describes the relations between the crystal axis system to the instrument axis system.

If you have centered 3 independent reflections with known hkl, you can calculated it based on the initial lattice constants. You even can refine the lattice constants. The program for this is called RAFIN and can be called by the command ubrefine in SICS. The new matrix can be loaded with ubload. Details are given on the intranet sites of ZEBRA (https://zebra.intranet.psi.ch).

```
Title is Nd2NiO4.125
2 1 0 0 25 3 4 1 .5 0     (25=minimal angle between basis reflections)
0  2.2149                            (wavelength, no refine)
0 .0 0 .0 0 .0                       (no refine of zeropoints)
1 5.39 1 5.40 1 12.34 0 90 0 90 0 90(1=refine, 2=dependent refine)
   0.0000    0.0000    6.0000   65.017   32.550    0.127   36.296
   2.0000    0.0000    0.0000   48.408   24.160   -1.477  126.300
   2.0000    0.0000    2.0000   53.185   26.609   -1.505  102.628
-1
```

Note: refinement of lattice constants is only possible by running it outside SICS by rafin >! Rafin.lis and loading it in SICS by ubload.
Literature: W.R. Busing, H.A. Levy, *Acta Cryst.* (1967). 22, 457

Indexing Reflections:

Idea behind the program: the angle between two reflections is known from the cell constants and can be compared to the measured angles between observed reflections.

You found at least 2 reflections and you know the cell constants: The program index can test all combinations. An example file is given in /home/orionlnsg/examples/index.dat.
You just type INDEX and on the first input request the number of reflections you want to use. Do not use more than 3 to 4, otherwise calculations time is exploding. The program is also explained further on the ZEBRA intranet sites.

```
sample Nd2NiO4+x (do not use more than 4 reflections)
5.38 5.45 12.35  90.0   90.0   90.0  2.21 3.5  (3.5: error accepted)
65.978   32.552    0.953   90.231 1.1       (1.1 is the error in 2Θ)
48.263   24.313   -1.728  130.575 1.1        (2Θ  ω φ χ ΔΘ)
0                                           (0: job end)
```

Note: your run this outside SICS by typing index and responding with 2 (number of reflections). Suggestion will be printed on index.lis

Ratemeter:

- Select range
- Select channel B at the counter box to be displayed (B=detector, A=Monitor)
- Integration time is unfortunately fixed (upgrade is in the LDM working list)

Command files:

For searching reflection, you can create command files, which can call themselves other command files.*Feedback is welcome anytime.* Jürg Schefer, Dec. 2015

Some hints for the SICS command to be used on ORION:

What you need: a,b,c,alpha,beta,gamma and a good crystal

mode bi
[bisecting mode for ORION, prefers CHI around zero compared to ZEBRA with CHI around 180^{o}]

cell a b c alpha beta gamma
enter cell parameters

lambda 2.2141

four
type all angles, stt, ch, pi and om

cscan stt start step number monitor
centrals scan of stt around start
“good ”steps: stt: 0.2, om: 0.05-0.15, ch: 0.3-0.5, ph: 0.05-0.15

peak
calculates the center of the last scan (does not move the instrument)

center
drives to the last center calculated

reflist
Makes a list of all reflection to be used for the UB

refsave ref.center
saves the list on the disk as ref.center

refclear
deletes this list

refadd idxang h k l
add the current postion to the list with index h k l

ubrefine
refines the ub

ubload
load the ub from file rafin.lis created in the projectdir directory. With rafin >! rafin.lis you can adjust the cell parameters by setting the flags before the parameters from 0 to 1 and load them with loadub

drive hkl [h] [k] [l]
drive to hkl with the present UB

angtohkl (optional: stt om chi phi)
calculates the hkl from the current position or the angles using the ub matrix

hkltoang h k l
calculates the position of reflection hkl (stt om chi and phi) using the ub matrix

calcstt h k l|

calculates 2-theta from the unit cell