

peakref

Introduction

- Refinement of unit cell parameters and orientation matrix
- Refinement of diffractometer parameters
- Constraints are available

help

- Typing “help” will open a webpage with the manual.
- Typing “help commandname” will open a webpage with the manual entry for the commandname.
Example: “help go3”

rmat

- The command “rmat” reads the orientation matrix from a file
- If the rmat-file contains information about the point group, constraints are set accordingly
- With the commands “rmat2”, “rmat3”, etc. It is possible to read additional orientation matrices

pk

- The command “pk” reads a file with the impact positions
- With the commands “pk2”, “pk3”, etc., additional files can be read
- If the pk-file originates from a peak-search, reflections are not indexed
- If the pk-file originates from an Eval15 integration, reflections are indexed

hklreind/reind

- By default, the program peakref does not re-index reflections
- With the commands “hklreind” and “reind” the user can change this behaviour

free/fix

- With the commands “free” and “fix” the user selects the parameters which are (not) refined.

status

- The command “status” shows the current values of parameters
- It also shows if a parameter is free or fixed

go

- The command “go” performs the refinement
- The command “go3” performs 3 cycles of refinement

byexperiment

- The command “byexperiments” allows the parameter to have a different value for every experiment (“scan”)

reject

- Largely deviating reflections are not used in the refinement (“forbid” flag)
- It depends on the average residues *resmm* (mm residue) and *resrot* (rotation residue). Deviating means $f * resmm$ and $f * resrot$
Example: reject 5 (this means $f = 5.0$)
- If the refinement improves, more reflections should fit
- On the other side, during refinement *resmm* and *resrot* become smaller. Therefore a smaller deviation will flag the reflection as “forbid”.

Saving results

- save: new file “dotalign.vic”
- savermat: new rmat-file
- save gonio: new file “goniostat.vic”

reportsigma

- The command “reportsigma” writes the current cell parameters and their standard uncertainties into the file *peakref.lis*