Very basic SPEC commands

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This document presents the typical ways to use some basic SPEC commands for a single-crystal diffraction experiment. An online manual can be found at http://www.certif.com and many topics are described in the help utility. SPEC is a (case-sensitive) command-line based program. Therefore it is important to know the correct commands; fortunately, some commands will list the type of parameters needed if the wrong type (or number) are entered.

“Information” and miscellaneous commands

pa
Lists parameters such as the orientation matrix, lattice parameters, operating mode, wavelength, etc.

wh
where; lists positions of the diffractometer motors, reciprocal lattice coordinates, and some relevant angles.

wa
where all; lists positions of all the SPEC motors (in user units and dial units).

p some expression
print; can be used to print a variable’s value:
p F_CHI
or as a calculator:
p 5*sin(PI/4)

help [topic]
calls SPEC’s help utility

cr [time]
counts and lists results for all scalers. The counting is for time sec or for the default time if value is omitted (such as 1 sec). But if value is negative, then counting continues until the monitor (a particular scaler) reaches value counts. Examples of use:
cr
cr 10
cr -100000

startup
Initializes a variety of parameters by calling the macros newsample, newfile, setsans, setplot, and setgeo. These semi-self-explanatory macros can also be called directly.

quit
quit out of SPEC.

Simple motor motions

umv motor_name position
move motor_name to absolute position (in user units). Examples:

umv th 20
umv th CEN
See below under dscan for information on the variable CEN.

umvr motor_name rel_position
move motor_name by the relative amount rel_position from its current position.

ubr H K L
move motors to the reciprocal lattice point (Bragg point) defined by the Miller indices H K L

cr H K L
calculate the motor position for the reciprocal lattice point H K L. It’s a good habit to do ca before ubr, to avoid unexpected motor motions.

tw motor_name delta
tweak; interactive subroutine to move motor_name by delta. Once in the subroutine, each time you hit Enter the motor moves by delta. You can change direction with p/n or +/-, and also change delta by entering a new value. Escape by hitting CTRL-C.

Basic scans

For scans in SPEC, one enters the number of intervals, which is one more than the number of points. Thus, the step size is (ending point) - (starting point)/intervals. The unit of time is seconds per point if positive, or monitor counts per point if negative.
loopscan npts [count_time [sleep_time]]
  time-lapse scan: sit and count for npts points without moving motors

timescan [count_time [sleep_time]]
  indefinite time-lapse scan

Motor scans

ascan motor_name start end intervals time
  absolute scan: motor_name starts at start and ends at end (in user units). At the end of the scan, motor_name stays at end. Example:
ascan th 5 7 30 1

dscan motor_name rel_start rel_end intervals time
  relative (differential) scan: motor_name starts at start + current_position and ends at end + current_position. At the end of the scan, motor_name returns to its previous position. This is the same as a lup (line up) scan. Example:
dscan th -1 1 30 1; umv th CEN

The variable CEN is calculated after each scan, and is the absolute position of the peak’s center. Note that if you typed umvr th CEN or umv phi CEN you could get into big trouble! It may also give weird results if there is no peak, or if the FWHM couldn’t be calculated from the scan.

a2scan motor_name1 start1 end1 motor_name2 start2 end2 intervals time
  absolute scan of two motors: motor_name1 starts at start1 and ends at end1, while motor_name2 starts at start2 and ends at end2. a3scan and a4scan operate similarly, d2scan, d3scan, and d4scan are multimotor relative scans.

mesh motor_name1 start1 end1 intervals1 motor_name2 start2 end2 intervals2 time
  motor mesh scan. A scan of motor_name1 is done for each point of motor_name2, all of which is stored as one SPEC scan. Example:
  mesh th 5 7 50 tth 10 14 30 1
  In this example, the full scan contains 51*31=1581 points.

Reciprocal space scans

hscan h_start h_end intervals time
  linear scan in reciprocal space along the H axis. The values of K and L during this scan are based on the previous position in reciprocal space, so you may need to use the ubr command to first move to the appropriate point. Example:
  ubr 1 1 1; hscan .9 1.1 20 2

kscan k_start k_end intervals time
  same as hscan but along the K axis.

lscan l_start l_end intervals time
  same as hscan but along the L axis.

hklscan h_start h_end k_start k_end l_start l_end intervals time
  linear scan in reciprocal space along a general direction. For example, if you wanted to scan in some direction along H and K thru the (111) Bragg peak:
hklscan .9 1.1 1.2 0.8 1 20 1

hklmesh Q1 start1 end1 intervals1 Q2 start2 end2 intervals2 time
  reciprocal space mesh scan. Q1 and Q2 are literally H, K, or L. Thus this type of mesh scan is limited to be along the principal axes of reciprocal space. The value of the third reciprocal space coordinate during this scan is based on the previous position in reciprocal space, so you may need to move there first. For example, if you wanted to scan in the H-L plane thru the (111) Bragg peak:
  ubr .8 1 .9; hklmesh H .8 1.2 20 L .9 1.1 20 1

Orientation matrix commands

With two nonparallel reflections entered into the orientation matrix, SPEC can perform the transformation between diffractometer angles and reciprocal lattice coordinates.

or0
  Sets the primary reflection, when you are at the appropriate angles.
or1
  Sets the secondary reflection, when you are at the appropriate angles.

setor0
  Sets the primary reflection by asking for the reflection’s angles.

setor1
  Sets the secondary reflection by asking for the reflection’s angles.

setlat
  Command to input the lattice parameters.

A few useful variables

LAMBDA: wavelength in Ångstroms
OMEGA: theta-(twotheta)/2
ALPHA: incident angle (typically)
BETA: exit angle (typically)
AZIMUTH: rotation angle of reference vector about scattering vector (may vary with geometry)