PRISMA Operating Program Manual

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Introduction

The PRISMA spectrometer is controlled by a Fortran program PRISMA operated from the PRSMGR instrument account by typing

```
PRISMA
```

at which point the prompt

```
PRS>
```

will appear. The program allows the user to drive or scan detector, analyser or sample angles, analyser or detector energies, and to position the spectrometer for an inelastic scattering measurement by specifying the direction of measurement in reciprocal lattice coordinates and the energy transfer to be measured at a specific point along the direction of the measurement.

Control Commands

A command line consists of a 2 letter command name followed by a space, followed by the list of parameters for that command. For some of the commands, PR, TI, DO, and VX only the parameter name need be provided. For some no parameter is needed (eg. BE and EX) but for most, SE, DR, SC, BR, and CD a format

parameter name = numerical value

is required. For the BR and CD commands, there exists a sense of order between the parameter values, and if that sense of order is followed only the numerical values need be entered.

PR <nn>	Print parameters
SE <nn> = xx	Set parameters
DR <nn> = yy	Drive motor/angles
SC <nn> = ct,st,NP = np	Scan motor/angles
BR QH = h,k,l,phi,dom,np	Bragg peak scan
CD QH = h,k,l,dh,dk,dl,en	Collect inelastic data
TI text string	Change run title
BE	Begin counting
DO file.job	Execute job file
VX C=command line	Perform VMS command
EX	Exit PRISMA control program

Unit conventions

Energies	meV
Scattering vectors	reciprocal lattice units
Flight times	microseconds
Flight path lengths	metres
Translation distances	centimetres
Angles	degrees
Lattice constants, d-spacings	Å

Spaces or commas may be used as separators.

Angle Names

The convention used to name the angles (motors) on PRISMA is as follows

A<nn>	PRISMA-2 analyser angle
D<nn>	PRISMA-2 detector angle
FRT<nn>	PRISMA-3 front analyser angle
BRT<nn>	PRISMA-3 rear analyser angle
TRN<nn>	PRISMA-3 translation distance
PHI<nn>	Scattering angle of analyser-detector arm
OM	Omega angle of the sample
GX,GY	Tilt angle of perpendicular goniometer arcs

The angles are displayed on a PC screen under the headings

ANA1 to ANA16
DET1 to DET16
FRT1 to FRT5
BRT1 to BRT5
TRN1 to TRN5
PHI, PSI, GX, GY

and are the same as those produced by the PRINT command.

The OM angle is defined in reciprocal space to be zero when the crystal direction PX is parallel to the direction of the incident beam. The zero angle ZOM relates these angles in reciprocal space to the "absolute" angle, PSI, which is where the goniometer is positioned, ie.

PSI = ZOM + OM

ZGX and ZGY are the zero angles corresponding to the two goniometer arcs.

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Parameter groups

There are 5 groups of parameters in the PRISMA program: the motor zero/limit parameters, the sample parameters, the analyser parameters and the time of flight parameters. Within each of these groups there is a sense of order (this is relevant to the SE command), eg. for the sample parameters the order is A,B,C, <AB, <AC, <BC, PX(1), PX(2), PX(3), PY(1), PY(2), PY(3) and the parameters are presented in this order, but there is no sense of order between groups.

Motor parameters

Z<nn>	Zero offset of motor nn
L<nn>	Lower limit of motor nn
U<nn>	Upper limit of motor nn

Sample parameters

A, B, C	Lattice constants in Å
<AB, <AC, <BC	Lattice angles in degrees
PX(1), PX(2), PX(3) PY(1), PY(2), PY(3)	Vectors defining the scattering plane

Analyser parameters

DD	d-spacing of the analyser crystals in Å d=6.71 for pyrolitic graphite d=5.6569 for germanium d=9.882 for mica
AH, AK, AL	Miller indices of analyser scattering plane (0,0,-2) for pyrolitic graphite (1,1,1) or (1,1,3) for germanium (0,0,-1) or (0,0,-2) for mica
DMIN, DMAX	First and last of the array of active analysers
IANAL	Default analyser. Some commands require a designated analyser which, if not expressly stated will use this default analyser
MOD	Scattering sense of the analysers MOD = +1: Scattering to the left MOD = -1: Scattering to the right (looking in the direction of the neutron beam) MOD=0: Corresponds to the straight-through position of the detector (2-axis mode of PRISMA)
FOCUS	Spectrometer configuration FOCUS = 0: PRISMA-4 FOCUS = 1: PRISMA-2 FOCUS = 2: PRISMA-3 FOCUS = 3: PRISMA-3 & PRISMA-4

Time Of Flight parameters

MNT	Type of monitor counting unit. MNT = 0: "Forever" (ie. until an END command is issued by the supervisor) MNT = 1: ISIS frames MNT = 2: Neutrons in the monitor MNT = -1: No counting. The spectrometer is positioned but does not count.
MNS	Size of monitor count. Either number of frames (MNT = 1) or number of neutrons in the monitor (MNT = 2)

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BIN	BIN = 1: Channels are specified in constant time steps BIN = n: n < 10. Permits n time channel boundaries separating regions with different time channel bins BIN = 0: Use channels specified in CHANGE program
START	Value where the DAE should start taking data in microseconds (BIN = 1)
STOP	Value where DAE should stop taking data, in microseconds (BIN = 1)
STOPn	Upper time channel boundary for region n (BIN = n)
STEP	Size of time channel (BIN = 1) bins in microseconds
STEPn	Size of time channel bins in microseconds between START and STOP1, or STOP(n-1) and STOPn (BIN = n)

Note:
START, STOP and STEP should be given in multiples of 31.25 ns. If this is not the case, the program will make slight adjustments to the user defined values, so that this condition will be fulfilled.

Time resolved parameters

EON	Switch on time resolved mode. EON = 0: Normal operation, time reolved mode over-ridden EON = -1,-2: Diagnostic modes EON = 1: Direct superframe mode EON = 2: Superperiod mode. Requires file `hardperiods.dat` in `INST_TABLES`
DELAY	Delay time for electric field on in microseconds (must be in steps of 10 microseconds)
DURAT	Electric field on time in microseconds (must be in steps of 10 microseconds)
SFRAM	Number of frames in a superframe up to a limit of SFRAM = 22
LWIN, UWIN	Lower and upper limits for "acceptance" window in microseconds. ISIS pulses should arrive every ~20000 microseconds within the acceptance window, ie. within 20000-LWIN and 20000+UWIN microseconds. If the ISIS pulses do not fall within this time window, the pulses are vetoed until ISIS is stable

Print

Print the present value of all the parameters or of a set of parameters.

pr	samp	Sample parameters
	zero	Zero offset values
	angl	Present angle positions
	limi	Upper and lower limits of angles
	anal	Analyser parameters
	tof	Time-of-flight parameters
	ef	Energy settings of the active analysers
	trs	Time resolved parameters
	all	Everything is printed

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or any combination like

```
pr anal samp
```

Set

```
se <nn>=x
```

All parameter changes which do not involve a positioning of a motor are performed with the set command. More than one parameter can be changed at a time.

```
se <ab=120,ianal=10,px(1)=0
```

If the order in a parameter string is kept, only the first parameter to be changed has to be named.

```
se a=6.38 6.38 6.38 90 90 90
```

will set a=6.38, b=6.38, c=6.38, <ab=90, <ac=90, <bc=90. The parameters which can be set are grouped as sample parameters, analyser parameters, etc. Note that there is a sense of order between parameters within a group, but not between groups.

Drive

```
dr <nn>=xx
```

Drive one or several angles to a new position.

```
dr brt3=-210.24
dr phi13=-56.66
dr frt2-5=207.30
dr brt3=210.24 om=-13.78
```

Before a drive command is executed, the program checks if either the upper or lower limits will be exceeded by the new position, and also checks that no clashing with neighbouring analyser-detector arms will occur. The sequence in which the motors will be moved is specified in the sequence of the command, so in the third example first motor D2, then D3, D4, and last D15 will be moved. Specifying D15-2 instead of D2-15 would move the motors in the reverse order. In the same way, the analyser energies can be changed.

```
dr ef1-5=9.0
dr ef5=7.4 ef3=5.5
```

Scan

```
sc <nn>=<centre>,<step>,np=<np>
```

Perform a scan of one or more angles

A scan of <np> points with step size <step> will be made for every motor centred around <centre>. All three input parameters have to be declared, whenever the scan command is used.

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```
sc brt5=210.0,0.2,np=21
```

This command will make the back rotation of arm 5 scan from 208.0 degrees to 212.0 degrees in 0.2 degree steps. Several motors can be scanned through the same angles at the same time, but the number of steps must be the same.

```
sc brt1-5=215.0,0.1,np=25
sc frt1-3=220.0,0.25,np=21
sc frt3-1=220.0,0.25,np=21
```

A combination of motors can also be scanned, eg. in a theta-twotheta scan

```
sc om1-16=40,0.1 phi1-6=40.0 0.2 np=17
```

In the same way, final energies can be scanned.

```
sc ef1-5=7,0.2,np=11
```

In an omega scan, the scattered neutrons will be counted in the analyser-detector arm that is specified by IANAL. Another detector can be chosen by writing the scan command in the following way

```
sc om5=34.6,-0.23,np=25
sc om13-15=-120.0,0.5,np=11
```

The neutrons will now be counted in detector 5 in the first example and in detectors 13-15 in the second. When scanning the other motors, the neutrons will be counted in the detectors associated with the scanned motors. In a scan command, as in a drive command, the program will check that no limits will be exceeded and that no clashing between neighbouring detector-arms will occur. If a clash situation does arise, the command will be aborted and a message printed. Sometimes it may be sufficient just to reverse the sequence of the motors to be moved, e.g brt3-1 instead of brt1-3. Note also that scanning an angle PHIn will automatically change the values of the other PHI angles as there is a fixed relationship between them.

Note:
Before launching a scan the TOF parameters will need to be changed to limit the amount of data collected and control the number of frames recorded at each step. MNT should be set to 1 (monitor type = frames) and the number of frames to be counted for should be set with MNS. The amount of data collected can be reduced by restricting the TOF window with the START, STOP and STEP parameters.

Bragg
```
br qh=<h>,qk=<k>,ql=<l>,phi=<f>,dom=<domega>,np=<n>
```

It is usual to leave out the qh= terms and to enter the command as

```
br -1 1 0 -80 0.2 21
```

The Bragg command will position the sample (omega angle) and the phi angle of detector IANAL so as to measure the Bragg peak (h,k,l) and its lower/higher orders in the diffractometer mode. If n > 1 an omega scan through the omega angle corresponding to this point will be performed with n points and an angular step domega (The time channel boundaries used will be those previously set with

START/STOP/STEP and the monitor type/size set with MNT/MNS). If n = 0 the spectrometer will just be positioned and no counting performed.

Collect data (CD)

```
cd qh=<h> qk=<k> ql=<l> dh=<dh> dk=<dk> dl=<dl> e=<en>
```

The command is usually entered without the qh= terms as

```
cd 1 1 2 0 0 1 3
```

This command starts an inelastic run where h, k, l determine a point in reciprocal space, dh, dk, dl give a direction in reciprocal space. These six parameters determine the direction in reciprocal space along which the data will be taken. The last parameter en determines the value of the energy transfer on the time of flight path belonging to analyser IANAL at the wavevector (h,k,l). These 7 parameters completely define the energy/wavevector transfer paths. The omega angle of the sample, the analyser and detector angles will be automatically positioned and the counting started by this command. This command will check that the detectors will not clash in the new configuration and will move them in an order so that they will not clash during the setting up of the configuration.

Note:
Check that the time of flight parameters MNT/START/STOP/STEP have been correctly set prior to issuing the CD command.

Title

```
ti <title of not more than 72 characters>
```

Change the run title shown on the instrument dashboard and stored in the raw file. There should be a single space between TI and the title, with all subsequent characters interpreted as the title. This command is useful for changing the title between runs contained in a jobfile invoked with the DO command.

Begin

```
be
```

Start a measurement using the current settings of the time of flight parameters, MNT/START/STOP/STEP.

Warning!
If you do not issue this command from the PRISMA operating program, the spectrometer angles, sample parameters and structure of the raw file described by the spectra.dat file will not be stored in the .raw file with the experimental data. It is very difficult to interpret data files without this information.

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Do

```
do test.job
```

Execute a job file.

The prompt on the LA120 will be changed to DO>> in order to indicate where the command came from. A job file is a file containing a list of PRISMA commands', one command per line, to run as a batch process. Note:
Do not include a prompt in the file before a command line.
Do not insert blank spaces at the beginning of each line.

Filenames for a DO command are limited to 10 characters each.
Nested DO files are not permitted

Exit

```
ex
```

Terminate the PRISMA operating program.

VMS command (VX)

Run a VMS system command line from within the PRISMA operating program.

```
vx c= <VMS command line>
vx f= <Filename of a file containing VMS command lines>
```

An example of the use of VX would be to change the temperature from within the PRISMA program

```
vx c=cset temp 100.25
```

There should be no space between the C, the = and the command line or file name, although spaces within a command line are allowed.

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