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The PRISMA Operating Program Manual

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Unit conventions:

Energies are given in meV.
Scattering vectors are given in reciprocal lattice units.
Flight times are given in microseconds.
Angles are given in degrees.
Lattice constants and d-spacings are given in Å.

Spaces or commas may be used as separators.

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Contents

1 Introduction

The PRISMA spectrometer is controlled from the LA120 terminal in the PRISMA cabin by running a program PRISMA. If the program is not already running then it can be started by logging in to the account PRSMGR on the LA120 and typing PRISMA, at which point the prompt PRS> will appear. The program allows the user to drive (move) or scan detector/analyser/sample angles and analyser/detector energies and to position the spectrometer angles (16 detectors, 16 analysers and sample) for an inelastic scattering measurement by specifying the direction of measurement in reciprocal lattice co-ordinates and the energy transfer to be measured at a specific point along the direction of the measurement.

The rest of this section is divided into two sub-sections, the first describes the names used for the different angles involved in defining the spectrometer configuration. The second describes the parameters used to define (i) the motor zero and limit angles, (ii) the sample, (iii) the analyser crystals and (iv) the time of flight channels. The next section describes the control commands in the program.

1.1 Description of Angle Names:

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

A$<nn>$	-	Analyser angles $<nn>= 1$ to 16.
D$<nn>$	-	Detector angles $<nn>= 1$ to 16.
PHI$<nn>$	-	ϕ angle (scattering angle) for analyser-detector system $<nn>$. $<nn>= 1$ to 16
OMEGA or OM	-	The omega angle of the sample.
GX,GY	-	The tilt angle of the two perpendicular arcs.

The angles D1-16,A1-16 and PHI01 are displayed on the P.C. screen under the headings DET1 to DET16, ANA1 to ANA16 and PHI. These angles should be the same as those printed by the PRint command. The angles OMEGA, GX and GY are displayed on the "dashboard" display under the names PSI, ANG1 and ANG2, which differ by the zero angles, ie;

$$PSI = ZOM + OM \quad ; \quad ANG1 = ZGX + GX \quad ; \quad ANG2 = ZGY + GY$$

where ZOM, ZGX and ZGY are the zero angles. The omega angle is defined in reciprocal space and is zero when the crystal direction PX (see sample parameters section) is parallel to the direction of the incident beam (k_i). The zero angle relates these angles in reciprocal space to the "absolute" angle, PSI, which is where the goniometer is positioned.

1.2 Description of PRISMA parameters:

There are 4 groups (or families) 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.

1.2.1 Motor parameters:

Z< *nn* >   zero offset of motor *nn*

L< *nn* >   lower limit of motor *nn*

U< *nn* >   upper limit of motor *nn*

1.2.2 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

1.2.3 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 fo 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; if not expressly stated otherwise, the program 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)

1.2.4 Time Of Flight parameters:

MNT   type of monitor counting unit.
MNT=0 is "forever" (ie. until an END command is issued by the supervisor)
MNT=1 is for ISIS frames
MNT=2 is for neutrons in the monitor
MNT=-1 does not perform any 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)

BIN   BIN=1: channels are specified in constant time steps
BIN=0: use channels specified in CHANGE program

START   value where the DAE should start taking data, given in microseconds (BIN=1)

STOP   value where DAE should stop taking data, in microseconds (BIN=1)

STEP   Size of time channel (BIN=1) bins in microseconds

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

2 The Control Commands

A command line typed on the LA120 (or in a jobfile) 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, VX and CSET only the parameter name need be provided, for some no parameter is needed ie., BE and EX, but for most, SE, DR, SC, BR, and CD a format parameter name = numerical value is required. For the two latter 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.

<u>List of commands</u>

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 job.file	: execute jobfile
VX C=command line	: perform Vax command
CSET	: set temperature logging
EX	: exit PRISMA program

2.1 The <u>PR</u>int command:

This command allows you to print the present value of all the parameters or of a set of parameters. The general form of the command is :

$$PR < nn >$$

with $< nn > =$	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
	ALL	everything is printed

or any combination like

$$PR\ ANAL\ SAMP$$

2.2 The <u>SE</u>t command:

The general form is :

$$SE < nn >= x$$

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, e.g.:

$$SE < AB=120, IANAL=10, PX(1)=0$$

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

$$SE\ A=6.38\ 6.38\ 6.38\ 90\ 90\ 90$$

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. These groups and the order of the parameters within the group is given at the end of these notes. Please note that there is a sense of order between parameters within a group but not between groups.

2.3 The <u>DR</u>ive command:

The general form is :

$$DR < nn >= xx$$

This command will drive one or several angles to a new position, e.g.:

DR	A10=12.34
DR	PHI13=56.66
DR	D2-15=23.45
DR	D3=60.89 A1=20.5 OMEGA=-13.78
DR	A1-4=45.0
DR	A11=45.0 A12=45.2 A13=45.4

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Before a drive command is executed, the program checks if either the upper or lower limits will be exceeded by the new position; the program also checks that no clashing with neighbouring analyser-detector arms will occur. Please note that 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 reversed order. In the same way also the analyser energies can be changed e.g.:

$$\text{DR} \quad \text{EF1-16}=20.0$$
$$\text{DR} \quad \text{EF7}=15.2 \text{ EF6}=15.0$$

2.4 The SCan command:

The general form is :

$$\text{SC} < nn >= ct, \; st, \; \text{NP} = np$$

This command will perform a scan of one or more angles; the scan will be centered for every motor around ct, the step size will be st and the number of points will be np. All three input parameters have to be declared, whenever the scan command is used. An example of the use of the scan command is :

$$\text{SC} \; \text{A6}=39.3,0.2,\text{NP}=17$$

This command will make analyser 6 scan from 37.7 degrees to 40.9 degrees in 0.2 degree steps. Several motors can be scanned through the same angles at the same time, only the number of steps has to be the same, for example ;

$$\text{SC} \quad \text{A1-10}=35.3,0.1,\text{NP}=35$$
$$\text{SC} \quad \text{A10-15}=30.2,0.25,\text{NP}=21$$
$$\text{SC} \quad \text{A15-10}=30.2,0.25,\text{NP}=21$$

Also a desired combination of motors can be scanned, eg. in a theta-2theta scan:

$$\text{SC} \; \text{A1-6}=20.0 \; 0.1 \; \text{D1-6}=40.0 \; 0.2 \; \text{NP}=17$$

In the same way final energies can be scanned:

$$\text{SC} \quad \text{EF1-16}=25,2,\text{NP}=19$$
$$\text{SC} \quad \text{EF12-5}=50,5,\text{NP}=11$$

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:

$$\text{SC} \quad \text{OMEGA5}=34.6,-0.23,\text{NP}=25$$
$$\text{SC} \quad \text{OM13-15}=-120., 0.5,\text{NP}=11$$

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 detector(s) associated with the scanned motor(s). In a scan command, like in a drive command the program will check before every new positioning that no limits will be exceeded and that no clashing between neighbouring detector-arms will occur. If a clash situation should arise, the command will be aborted and a message will be printed. Sometimes it may be sufficient just to reverse the sequence of the motors to be moved, e.g D3-1 instead of D1-3.

Please also note that scanning an angle PHIn will automatically change the values of the other 15 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.

2.5 The BRagg command:

The general form is :

$$\text{BR QH} = \text{h, QK} = \text{k, QL} = \text{l, PHI} = \phi, \text{DOM} = d\Omega, \text{NP} = \text{n}$$

although it is usual to leave out the QH = terms and to enter the command as :

$$\text{BR h, k, l}, \phi, d\Omega, \text{n}$$

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 $d\Omega$. (Note the time channel boundaries used will be those previously set with START/STOP/STEP and the monitor type/size that with MNT/MNS). If n = 0 the spectrometer will just be positioned and no counting performed.
Examples;

$$\text{BR} \quad 1\ 1\ 1\ \text{-90}\ 0\ 0$$
$$\text{BR} \quad \text{-1}\ 1\ 0\ \text{-80}\ 0.2\ 21$$

2.6 The CD command:

The general form is:

$$\text{CD QH} = \text{h QK} = \text{k QL} = \text{l DH} = \text{dh DK} = \text{dk DL} = \text{dl E} = \text{en}$$

although the command is usually entered without the QH = terms as :

$$\text{CD h k l dh dk dl en}$$

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. (Note the time of flight parameters MNT/START/STOP/STEP should have been accordingly set prior to issuing the CD 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.

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2.7 The DO command:

The general form is :

<div align="center">DO TEST.JOB</div>

This command executes 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, which are to be run "in batch". The same sort of idea as a DCL .COM file. Note there is no prompt to be included in the file before a command line and the commands should be left adjusted (no blank spaces at the beginning of the line !!). The filenames for a DO command are limited to 10 characters each. Note you cannot DO a file from within a jobfile.

2.8 The TItle command:

The general form is :

<div align="center">TI title of not more than 72 characters</div>

This command allows the user to change the run title (as shown on dashboard and stored in the raw file). There should be a single space between TI and the title, apart from that everything else on the line will be interpreted as the title. This command is useful for changing the title between runs contained in a jobfile and run with a DO command.

2.9 The BEgin command:

The general form is :

<div align="center">BE</div>

This command can be used to start the spectrometer counting. The advantage of issuing a begin from the PRISMA program rather than the supervisor terminal is that the angular positions/sample parameters/spectra.dat etc. are stored in the raw file, which they aren't if the begin comes from the supervisor. Note the time of flight parameters MNT/START/STOP/STEP used will be those that have been set previously.

2.10 The VX command:

This command can be used to run a Vax system command line from within the PRISMA program. It has two forms :

<div align="center">VX C= Vax command line
VX F= filename of a file containing Vax command lines</div>

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

<div align="center">VX C=CSET TEMP 100.25</div>

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

2.11 The CSET command:

There is a difficulty with the CAMAC control software on ISIS instruments whereby when moving a motor and logging temperature at the same time it is possible for the motor control command and the log value of the temperature to become interchanged, ie. temperature is sent to angle and angle to temperature ! To avoid this it is necessary to switch off temperature logging while moving a motor. The PRISMA program will do this automatically if (only if) the temperature logging command was set in the PRISMA program. The general form of the command is :

CSET se_block/log_control

where the possible se_block parameters are TEMP, TEMP1 and LAKES (the Lakeshore controller) and the log_control values are LOG and NOLOG. Note the CSET should be left adjusted, just one space between CSET (all 4 letters) and the se_block name, no spaces between the se_block name, the / and the log_control value. It is intended in the future to extend the CSET command to allow the normal setting of CAMAC values from within the PRISMA program but for the time being this must still be done using the VX command.

2.12 The EXit command:

The general form is :

EX

This command terminates the PRISMA control program.