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DATA ACQUISITION SOFTWARE AND ELECTRONICS ON THE ENERGY-DISPERSIVE POWDER DIFFRACTION STATION 9.7

by

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Data acquisition software and electronics on the energy-dispersive powder diffraction station 9.7

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Abstract

This report describes the data acquisition electronics and computer software in use on the energy-dispersive powder diffraction facility at the SRS. It is intended as a guide and source of information for users of the facility as well as a complete description of the electronics and computer software currently employed.

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1 Introduction

Station 9.7 of the synchrotron radiation source (SRS) st the Daresbury laboratory houses the energy-dispersive powder diffraction facility. This is used to study the properties of materials under extreme conditions such as high temperature or presure, and to follow chemical reactions. The experiment uses very hard X-radiation and for safety reasons has to be housed remotely from the experimentallist. This means that all equipment must be remotely controled with motions provided by motors. A large range of experiments are carried out on the station with users visiting for a few days at a time. The system has to be flexible enough to allow rapid changes in line with current experimental needs as well as simple enough to allow outside users to use the facillity with the minimum of training. This report describes the station electronics and data acquisition software currently in use on station 9.7.

2 Description of the station electronics

The station electronics can be divided into three parts: the detector and monitor counting chains, ion chamber counting chains and stepper motor electronics. All of these are controled, via CAMAC, by the station computer (figure (1)). The station electronics are mainly of two types: CAMAC (figure (2)), and NIM (figure (3)). All of this equipment is kept in cabinets outside of the experimental enclosure and connected to the equipment inside of the enclosure via two interface boxes. One interface box has connectors for stepper motor cables and the other has a range of connectors including BNC, SHV and CANNON (figure (4)). An amount of excess capacity has been allowed in the station design to allow users to add their own electronics or stepper motors.

2.1 Counting chains

There are two identical counting chains in use on station 9.7; one for the semiconductor detector and the other for the monitor. The monitor may be either a scintillation counter or a semiconductor detector; the only difference, as far as we are concerned here, is that the scintillation counter opperates at a voltage of +800V whereas the semiconductor detector operates at -1500V.

The semiconductor detector (EG&G GLP-06165/05) consists of a germanium crystal with electrodes attached to the front and back with a high reverse bias voltage (-1500V) applied across them. Photons interact with the crystal and produce electron hole pairs. These are swept to the respective electrodes by the electric field. The resultant charge is integrated and converted to a voltage pulse that is proportional to the incident photon energy by a charge sensitive preamplifier. This signal then goes to a EG&G 572 amplifier which amplifies and shapes the pulse. Output from the amplifier is passed to a LeCroy 3512 buffered ADC coupled to a LeCroy 3588 histogramming memory module. The ADC accepts voltage pulses from 50mV to 8V and maps them on to 2000 or 4000 channels. The upper and lower voltage levels and gain on the amplifier can be varied to select the range of photon energies of interest. The ADC constructs a channel address derived from the input voltage level. This address causes the channel in the histogramming memory to be incremented directly. The histogramming memory can be read without halting data acquisition so that spectra can be displayed on the terminals as they are collected without adding any overhead to the data acquisition time. The detector and monitor are powered by two Ortec 459 bias supplies. The monitor by bias supply (1) and the detector by bias supply (2) (figure (3)). These are connecterd by wires P1 and P2 through SHV connectors 1 and 2 in the interface box (figure (4)). The detector preamplifier is powered by a supply in the Ortec 572 amplifier. This is connected from the back of the amplifier via nine pin canon 9A of the interface board to the detector preamplifier. The detector remote bias shut down is connected to the Ortec 459 power supply via BNC3 of the interface board. The detector and monitor signals are carried directly from the inside of the experimental enclosure to the Ortec 572 amplifiers by cables Sig1 and Sig2.

2.2 Ion chambers

Ion chambers are power by a Ortec 456 high voltage power supply set to +700V. This may be connected to up to two ion chambers by the wires marked I1 and I2. The other side of the ion chamber is then connected to one of two Keithley current to voltage amplifiers by cable IS1 or IS2. The outputs of the Keithley amplifiers are connected via BNC1 and BNC2 of the interface box (figure (4)) to an EXAFS current monitor outside of the hutch. IS1 on the left hand monitor and IS2 on the right. The signals also pass through a voltage to frequency (V-F) converter to a quad counting register from which they are read by the computer (Figure (5)).

2.3 Station computer and timing electronics

At the center of the station electronics is a LSI 11/23 computer. This is connected via CAMAC to the data acquisition electronics, stepper motors and a site wide ethernet network.

A Hytec 95 pulse generator is used to provide pulses at 1 kHz to time the period of data collection. This is gated with a DL EC524 Scaler/inhibitor to synchronise the counting. The counting time is predefined such that a register overflow occurs in a Hytec 350A quad counting register when the preset limit is reached. The sequence of operations for

data collection is:

1. The computer loads the time for data aquisition into the quad counter.

2. The computer enables data collection by sending a command to the scaler/inhibitor.

3. The computer enables the Le Croy ADC and histogramming memory for data collection.

4. Data collection proceeds. The spectrum is plotted on the computer terminal every two seconds.

5. The quad counter overflows and causes the scaler/inhibitor to inhibit further counting and the ADC and histogramming memory to halt data collection.

The values stored in the four registers of the quad counting register are written into a file together with the collected spectrum on the hard disk. Normally the second register is used to record the system dead time (By connecting the busy out from the ADC to it) and the third and fourth registers to record ion chamber readings. One may also inhibit data collection using these other registers, so for example collect spectrum for fixed incident flux.

2.4 Stepper motors

All of the motions on station 9.7 are provided by stepper motors. To drive a motor the computer loads the stepper motor multiplexer with the address of the motor to drive, the number of steps to be taken, the step direction and the start/stop, acceleration, and maximum speeds. Each motor drive has a unique address set by eight switches on an highway interface module. The motor drives supply fixed current pulses to the motors, and are tuned to the loading and characteristics of each motor. Stepper motor drivers are connected into the hutch via a interface box. The wires and sockets are labelled from 1 to 20 and connect to the motors as labelled in table (1). Inside the hutch the connectors and cables are labelled in exactly the same manner. The wires inside the hutch connect to the motors via three types of connector: nine or fifteen pin canons and vax connectors. This is intended as a saftey measure: the CD20s and CD30s are connected to vax connectors, the LD2s to nine pin canons and the TM162Cs to fifteen pin canons.

2.5 Other electronic units

A number of units have already been added to the basic station electronics to meet specific user requirments. A Schlumberger JR10 interupt/alarm register for use in nucleation experiments, a Sension 1204 ADC for temperature input, and a EC727 24 bit multichannel scaler for multiple SCA inputs (up to 32), have been added.

There is also a TV camera inside the experimental exclosure connected via BNC9 of the interface box (figure (4)) to a TV screen outside of the enclosure as well as a TV screen inside the enclosure.

3 Description of the station software

The station computer is a 16-bit LSI-11/23 minicomputer running the DEC RT-11 V5.3 operating system. Data acquisition software is written in Fortran IV, and uses the CAMAC Modular Instrumentation and Digital Interface System (ANSI/IEEE standard 583-1982). The computer to CAMAC interface is a Sension 4510 Q-bus termination card extending to a Sension 1536 CAMAC crate controller. Software access to CAMAC uses standard Fortran-callable subroutines (ANSI/IEEE std. 758-1979, reaff 1981) written in Macro-11 assembler.

All the software is menu-driven, and has the standard SRS data acquisition group user interface based on extensive software libraries. Each program is heavily overlayed to bypass restrictions in the total low memory of 32Kwords. In some cases, non-standard virtual arrays are used to take advantage of the additional 96Kwords in high or extended memory. There are four programs that are run on the computer, two general purpose programs (DEDS and TOP) used for routine data collection and sample allignment, a data collection program tailored to a specific user need (TOMO), and a file transfer program (TFILE) that is used to transfer data files from the station computer to the laboratory mainframe (convex) computer where they are saved in a database ready for analysis.

3.1 DEDS program

The DEDS (Differential Energy-Dispersive Spectroscopy) program is the routine data acquisition program used on station 9.7. The program can collect two spectra simultaneously, one from the detector chain and one from the monitor chain. Either of these can be designated as the current spectrum. The current spectrum is the spectrum that is operated on by any commands, for example the DISPLAY command will display the current spectrum. Spectra can be collected using either a 2000 or 4000 channel range of the histogramming memory to map the data to, and can be written to disk in either ASCII or binary formats. Spectra can be collected individually or as a time sequence. The program is

started by command DEDS at the station terminal. A menu containing possible commands is displayed on the screen. The program is operated by entering commands, possibly followed by parameters, at the terminal. The following commands are currently supported:

HELP Synonyms H HE HEL HELP

Options	*HELP*	*LIST_DATA*
	PROCESS	*READ_DETECTORS*
	AUTOSCAN	*SAVE_DATA*
	FASTSCAN	*TOGGLE*
	NEWRUN	*QUIT*
	DISPLAY_DATA	

Information about commands can be displayed on the station terminal by giving the HELP command. Information about a specific command can be accessed by typing HELP COMMAND. HELP ALL displays information on all available commands.

PROCESS Synonyms P PR PRO PROC

The process command causes accumulation of data in the histogramming memory modules. Any data in the current spectrum is plotted on the station terminal every two seconds; giving a real-time picture of data as they are collected. On giving the process command the user is asked to give limits for the plot, pressing return gives the default values that are shown. The program then draws a frame for the plot and asks for the data acquisition time. Data is now accumulated in the histogramming memory modules and the current spectrum is displayed on the screen. When the specified time limit is reached the user is again prompted for the data acquisition time. To exit from the process command press CNTL_A either during data acquisition or when asked for the data acquisition time.

In order for spectra to be optimised during data collection, some motor driving capability is present in the DEDS program. The keys 1 to 8 of the station terminal drive motors as specified by menu A in the MOVE section of the TOP program. If a key is pressed, the motor moves by an increment determined by the motor parameter file. The direction of movement can be reversed by pressing SHIFT together with the motor key.

AUTOSCAN Synonyms A AU AUT AUTO

This command is used to collect a series of spectra. The user is asked for the data collection time and the number of scans to be carried out. The program then collects a sequence of spectra and saves each of them to disk. The information saved depends on the type of data set specified for saving; if OTOKO format is specified then both the monitor and detector spectra are saved but if SRS format is specified then only the detector spectrum is kept. In order to speed up data collection no graphical display is shown during data collection, only a note of the scan number. The sequence of scans can be aborted by pressing CNTL_A.

FASTSCAN Synonyms F FA FAS FAST

This command is like the AUTOSCAN command except that instead of writting data to disk in between scans, the data are stored in high or virtual memory of the LSI. This means that data can be collected with only a few milliseconds of dead time in between scans but only a maximun of sixteen scans of 2000 channels, or eight of 4000 channels, can be performed. After giving this command the user is asked for the time of data collection of each scan in milliseconds and the total number of scans. Data collection can be aborted by CNTL A.

NEWRUN Synonyms N NE NEW NEWR

This command clears both Histogramming memories and sets the accumulated count time to zero. If a memory module is not present an error message will result, but should be ignored unless you are using two memory modules. This command is given automatically when first starting the program.

Remember to copy any data that you want to keep for future analysis from the histogramming memory to the computer disk with the SAVE DATA command before erasing it from the histogramming memory unit with the NEWRUN command.

DISPLAY_DATA Synonyms D DI DIS DISP

This command reads the contents of the Histogramming memory specified by the current spectrum and displays the data on the station terminal in graphical form. This is the same display as is seen during PROCESS.

LIST_DATA Synonyms L LI LIS LIST

This command reads the contents of the Histogramming memory specified by the current spectrum. It displays the data on the terminal as it would appear in a SRS data file except for the namelist header which is obmitted. To stop the display type CNTL_A.

READ_DETECTORS Synonyms R RE REA READ

This option monitors the counts accumulating in registers one two and three of the quad counting register. The user is prompted

for a count time in seconds, after the specified period has elapsed the number of counts accumulated in each register is displayed on the station terminal. This command is particularly useful when checking that the gain on the Keightly amplifiers is set at the correct level.

SAVE_DATA Synonyms S SA SAV SAVE

Use this command to save data in the current spectrum histogramming memory module to a file specified by the default data file type (both settings displayed by the main menu). If OTOKO output is specified then two files are made: one is a binary file of about 16 blocks and the other is an ASCII header file which describes the format of the data file and has the quad counter values divided by 1000 as a comment field. With SRS data a single ASCI file containing the data is written to the disk, and should occupy about 76 blocks (~ 33 kbytes) when collecting in 4000 channels.

The file will be named **R <runnumber>.DAT**.

TOGGLE Synonyms T TO TOG TOGG

This allows default settings for some of the program parameters to be altered. To change any other parameters contact the Station master.

Options DATA SPECTRUM

DATA Switches the type of output data file between binary OTOKO format with associated ASCII descriptor file and ASCII SRS MCA dataset containing no line numbers.

SPECTRUM Switches the current spectrum between histogramming memory number 1 and number 2. This defines which histogramming memory is accessed by the PROCESS, AUTOSCAN (when SRS data is chosen), SAVE and LIST commands.

QUIT Synonyms Q QU QUI QUIT

Use this command to leave the program. It will bring you back to RT-11 command level.

All commands abort on typing CTRL_A.

3.2 TOP program

The **TOP** (**TOP**ography) program is a general purpose program developed at the Daresbury laboratory for data acquisition. The program is started by typing the command TOP. The program displays a menu containing the following commands:

HELP	*CHAIN*	*DISPLAY*	*INPUT*	*SET*	*QUIT*
MOVE	*EXPOSE*				
SCAN	*PLOT*	*MONITOR*	*SAVE*		
MULTIMOTOR					
SWEEP					

Because of the memory limitations of the station computer the TOP program has been divided into five physically distinct units which are chained together. The commands listed above are grouped horizontally into the differrent chains, which are known as the MAIN, MOVE, SCAN, MULTIMOTOR and SWEEP chains. The appropriate program unit is loaded into the station computer when a command is given. This version of the TOP program is menu driven. Option selection and parameter value changing is done by issuing a command line at the terminal that may contain a command, subcommand and values. Submenu options and values may be selected in the same way except for MOVE submenu options where the depression of a key without pressing RETURN starts execution. Commands and subcommands are carried over from one chain to another as well as numeric values issued in the same command line. Default parameter values are saved in a file which is read every time a chain is entered, restoring any scan parameters that were previously set.

All commands should be given in uppercase.

3.2.1 MAIN chain

HELP Synonyms H HE HEL HELP

Options		
	HELP	*EXPOSE*
	CHAIN	*SCAN*
	DISPLAY	*PLOT*
	INPUT	*MONITOR*
	SET	*SAVE*
	QUIT	*MULTIMOTOR*
	MOVE	*SWEEP*

Information about commands can be displayed on the station terminal by giving the HELP command. Information about a specific command can be accessed by typing HELP COMMAND. HELP ALL displays information on all available commands.

CHAIN Synonyms CH CH CHA CHAI

This command allows you to chain to another program installed on the stations disk. No programs are currently available to be run with this command.

DISPLAY Synonyms D DI DIS DISP

Lists the values of one of the following options:

MOTOR positions Synonyms M MO MOT MOTO

Positions are given in appropriate units for given motor, i.e., Degrees, Millimetres, or steps. Each motor is associated with a gearing ratio which converts between units to steps actually driven. Gearing ratios may be inspected using this command but can only be changed by the station master.

INTENSITY Synonyms I IN INT INTE

Lists continuously the beam intensity as measured by a reference Ion Chamber and the intensity recorded in a detector situated in the hutch. Integration time is in seconds. Use CNTL_A to end and return to the main menu.

EDGE INFORMATION Synonyms E ED EDG EDGE

Displays the absorption edge position in Angstrom and eV for a given chemical element and edge type (K, L1, L2, L3).

INPUT Synonyms I IN INP INPU

This command switchs command input from the station terminal to a file on the computer disk. Commands in the file are executed as soon as the file is selected and control returns to the keyboard after the last command in the file has been executed. The input file is closed when moving from one chain to another, so it can only contain commands that are grouped together in the same chain.

The MOVE menu only allows one key to be selected at any time the buffer is deliberately disabled for safety reasons hence problems will be encountered when using functions from this menu.

SET Synonyms S SE SET

This command is used to reset the absolute position of a motor. The motor names and positions are displayed on the screen. The up and down arrows are used to move to the appropriate line before entering the desired value.

QUIT Synonyms Q QU QUI QUIT

This command is used to exit the program and return to RT-11. Program parameters are saved to a file before exiting the program and are read in by the program when it is restarted.

3.2.2 MOVE chain

MOVE Synonyms M MO MOV MOVE

This command loads the MOVE chain into the computer and then asks which MOVE menu to display. Currently there are only two MOVE menus set up: one for powder diffraction (menu A) and the other for Laue diffraction (menu B). After typing A the powder diffraction MOVE menu is displayed. It is possible to set up MOVE menus customised for each user group and more MOVE menus will probably be added in the future. Table (2) contains a summary of the powder diffraction MOVE menu.

The status of active motors is continually updated on the station terminal and TV screen. Active motors may be stopped by either pressing the same function key or one of the PANIC buttons (Z or SPACE). If the PANIC button is used all further action is disabled until Z is pressed. The RETURN key will return control to the main menu. Motor positions are saved to a disc file after each movement but not during a movement. Before you move a particular motor check that the default speed and number of steps displayed on the top of the menu are the required ones. Positive steps move motors anticlockwise, negative steps move motors clockwise. The MOVE_TO or MOVE_BY options allow you to select motor and position first while the other motor keys start the motor immediately the key is pressed. Once a key is depressed all other keys are disabled until that operation is completed. Repressing the key will stop the motor moving, as will Z or SPACE.

The MOVE menu commands are:

M Move a selected motor to a given position. The program asks for a motor to be selected and then for a position to move to. It is necessary to press RETURN after giving the position.

N Move a selected motor by a number of steps. The program asks for a motor to be selected and then for the number of steps to move. It is necessary to press RETURN after giving the number of steps.

P Plate change. Moves a fixed number of steps in one direction.

I Read monitor and signal intensity. A time period is given, in seconds, over which the pulses from the monitor and signal detectors are counted. Press CTRL_A to stop counting.

S This command is used to set the number of steps that will be moved when a motor key is pressed. A positive value moves

the motor anticlockwise and a negative value moves the motor clockwise.

W This command allows a motor to be moved with the intensity automatically monitored at the end of the movement. The time interval is the same as the last time the INTENSITY function was used. Use CTRL_A to stop counting, and use W to cancel the function.

V Toggle the motor direction between clockwise and anticlockwise. Clockwise is equivalent to negative steps and anticlockwise is equivalent to positive steps.

X Set a motor speed to Fast, Medium or Slow. The Fast and Slow speeds are chossen by the station master, and the medium speed is the average of the two. The value in steps/sec is displayed in the MOVE menu heading while the motor is moving.

Motor speeds can be changed in the SCAN, SWEEP and MULTIMOTOR chains. If a value has been altered and does not coincide with the preset value then the speed is flagged as USED. This may not be the most appropriate speed for the motor.

Y Set the clockwise or anticlockwise software limit to the current motor position. These limits are software limits only, and are set by the user. They are displayed on the TV screen with the current motor positions. If a movement necessitates driving past a limit the user is asked whether to override the current limit; in that case the new final position becomes the new limit.To set the limits move the motor to the required position, press Y and enter clockwise or anticlockwise when asked.

L Lock, disables further movement for given motor.

U Unlock, enables movement of a given motor. The initial locked or unlocked state of each motor is defined in the configuratiion file.

AUTO This command switchs command input from the station terminal to a file on the computer disk. Motor movement may still be aborted by CNTL_Z, this also closes the input file and returns control to the station terminal. Should the commands in the file lead to lead to a situation where OVERRIDE or LOCKED prompts need answering then these prompts must be answered at the keyboard and not in the file.

Z Panic stop. Disables all functions. Press Z again to continue.

RETURN Return to main menu.

SPACE The station terminal space bar is used as a panic stop. It disables all functions. Press Z to continue.

EXPOSE Synonyms E EX EXP EXPO

Opens the shutter for an exposure. The exposure time, in seconds, may be given in the same command line. The default value is one second. Please note that the accuracy of exposures may be compromised by program speed for times less than one second.

There is currently no experimental shutter fitted.

3.2.3 SCAN chain

SCAN Synonyms SC SCA SCAN

This command initiates a motor scan. Any motor may be scanned by selecting the appropriate key when prompted. There are three types of scans: a centered scan, a forward scan and a straight scan. Each type of scan may be operated either normally, step then count, or as a FLYSCAN, count while stepping. In each type of scan the motor positions, and the values in quad counting registers one, two and three are saved in a temporary data file called the current spectrum file. The quad counting register three may be listed or plotted on the station terminal. contents of the current spectrum file may be saved to a file using SAVE, listed on the station terminal using DISPLAY_DATA, or plotted using PLOT. A scan may be aborted at any point by typing CNTL_A

1. **Centred scan** This performs a scan centred on a chosen position (START). The selected motor is moved to postion START-NSTEP*STEP, and is scanned to position START+NSTEP*STEP and then returned to position START. Only a start position and range are given when FLYSCANing.

   Backlash is taken up at the beginning and end of the scan.

2. **Forward scan** The selected motor is scanned from position START to position START+NSTEPS*STEP and is then returned to position START. Only a start position and range are given when FLYSCANing.

   Backlash is taken up at the beginning and end of the scan.

3. **Straight scan** The selected motor is scanned from position START to position START+NSTEPS*STEP and left there. Only a start and finish position position is given when FLYSCANing.

   No backlash is taken up.

Some parameters have to be set before a scan can proceed. A menu of parameters with default values is displayed by the program; they

may be altered by positioning the cursor in the appropriate line, using the up and down arrow keys, and then entering the new value.

START Defines the start position of the scan except for centred scan where this defines the middle position.

STEP Defines the step size. Positive values give anticlockwise motor movement and negative values clockwise movement.

NO OF STEPS Defines the number of steps (NSTEP) to be made between position START and position END. Position END is equal to START+NSTEPS*STEP.

END End position for flyscan.

NO OF SCANS Defines how may times a scan is to be repeated without resetting the scan parameters.

TIME_LIMIT Defines the count time, in seconds, at each point. In FLYSCAN motor movement is continuous; TIME_LIMIT and motor speed determines the number of steps moved between data points.

REF_LIMIT The Reference channel counting limit.

SIG_LIMIT The signal channel counting limit.

PLOT This toggles between either a plot or a list of data values appearing on the station terminal during the scan.

GRAPH_LOW This sets the minimum y-axis value for any graph ploted on the screen.

GRAPH_HIGH This sets the maximum y-axis value for any graph ploted on the screen.

STOP_LOW This sets a minimum count rate. The scan is stopped if the measured count rate falls below this value. This can be used as to monitor beam loss.

STOP_HIGH This sets a maximum count rate. The scan is stopped if the measured count rate goes above this value. This can be used to stop the detector from being driven into the direct beam.

SPEED This can be used to set the motor speed.

PLOT Synonyms PL PLO PLOT

The PLOT command is used to plot data from the current file, or a named file, to the screen. The PLOT command in the MAIN, SCAN and MOVE chains applies to data files created by the SCAN or MULTIMOTOR commands. The PLOT command in the SWEEP chain applies to data files created by the SWEEP command (two dimensional binary data). To plot one dimensional data created by the SWEEP command you need to be in the SWEEP chain.

MONITOR Synonyms MON MONI

This command monitors channels 2 and 3 of the quad counting register. Values can be plotted or written on the station terminal. Channel 2 is plotted as points and channel 3 as crosses. A time limit for each point is requested and then the elapsed and physical time and the quad counter values are recorded in the current data file. This may be SAVEd or PLOTted as for scan data.

SAVE Synonyms SA SAV SAVE

Saves the current data file as either:

1. **A SRS dataset** This is a file formatted according to the conventions adopted by the SRS Rapport database. A SRS dataset contains the run number, the date, the time of creation, a title, some optional comments and the data.
2. **Any other named file** The data is written in ASCII records, in the same form as for SRS datasets but without the header. These files can not be archived by the SRS Rapport database.

3.2.4 MULTIMOTOR chain

MULTIMOTOR Synonyms MU MUL MULT

Initiates multimotor scans. You are requested to select the number of motors (1, 2 or 3) and scan parameters as for the SCAN option. Any combination of motors may be scanned by selecting the appropriate key when prompted.

Parameter values are as defined in the SCAN routines.

Unlike the SWEEP command, the motors specified are moved by the predefined step value and then data is collected for time interval defined. Thus this scan is a one dimensional scan, where counts are collected for each channel and where each channel corresponds to new positions for the motors scanned. In all other respects this type of scan is like a straight one dimensional scan. The positions of the motors are written in the data file which may, at the end of the scan, be saved to an SRS dataset or a user named file. Backlash is taken up for each motor at the start of the scan.

3.2.5 SWEEP chain

SWEEP Synonyms SW SWE SWEE

This program is used for a special type of multimotor scan. A motor is scanned repeatedly while one or two other motors are steped by one step between each scan. The end result is a two or three dimensional scan.

You are requested to select the number of motors (1, 2 or 3) and scan parameters as for the SCAN option. Any motor may be scanned by selecting the appropriate key when prompted.

The main difference from the SCAN option is that the data points are saved in a direct access binary file of OTOKO format. For three dimensional scans a new file is opened every time the third motor is moved.

In order to reduce the total scanning time the leading motor position is neither displayed on the station terminal or saved to disk unitl the end of each leading motor scan. If the program crashes during a scan leading motor position mst be recalibrated using the SET command.

3.3 TOMO program

The TOMO program was written for a specific user need. The following commands are available:

HELP Synonyms H HE HEL HELP

Options	*HELP*	*ALL_HELP*
	NUCLEATION_RIG_SCAN	*TOMOGRAPHY_SCAN*
	READ_DETECTORS	*REPEAT*
	QUIT	

Information about commands can be displayed on the station terminal by giving the HELP command. Information about a specific command can be accessed by typing HELP COMMAND. HELP ALL displays information on all available commands.

All commands can be aborted by typing CTRL/A.

NUCLEATION_RIG_SCAN Synonyms N NU NUC NUCL

This SCAN is exactly the same as that of the "TIM" program. It has been superseded by TOMO as it is only occassionally used compared to Tomography work, but is in the same class of specialised application which requires it to be in a sepparate program from DEDS.

The data in the scan is the time taken for a diffraction peak integrated count to reach a predefined limit. The count is obtained from a Single channel analyser (SCA) which inputs pulses into channel 2 of the quad counter. Channel 1 measures the elapsed time from the start of the scan (in milliseconds). The scan starts when the user provides a trigger pulse (TTL logic) to release the sample into the

Nucleation Rig and signals to the JIR10 Interrupt Alarm CAMAC module that data collection is to proceed.

The user is prompted for the SCA count limit required (between 1 and 8 million). After this the program waits for the start trigger to be pressed before measuring the elapsed time before the SCA count is reached. During this time, CTRL_A will abort the measurement.

When Nucleation is complete, the program writes all the quad counting channel data to the screen and an output file TEMP.DAT. The user is then returned to the main Menu.

TOMOGRAPHY_SCAN Synonyms T TO TOM TOMO

In this measurement, a sample is scanned in the X-stage and the Y-stage axes to follow up to six diffraction peaks via six single channel analysers (SCAs). A two dimensional matrix is built up which is displayed on the screen as collected and written to either an **SRS** datafile or a temporary file TEMP.DAT (which will be overwritten by subsequent scans).

A number of parameters must be input by the user. Firstly the dwell time in Seconds (minimum 0.001) will specify the data collection period for the quad counter (QCR) detectors and the six SCAs (EC727 Multichannel scaler inputs) at each motor coordinate X,Y position in the scan. Next the start, step and no. of steps for X and Y must be specified. The positions are those seen in the TOP program Move Menu. If the step size for X and Y is set to 0 the motors will not move after being driven to the start positions and the number of steps for X and Y will allow the SCAs to be continually monitored (no. of times counts monitored = (No. of xsteps + 1) * (no. of ysteps + 1).

With valid parameters, the user then specifies either an **SRS** datafile or a TEMP.DAT file for the saved data. CNRL_A will abort the scan at any time when pressed with no loss of data collected so far.

The motors are driven to the start position which has the coordinates (X,Y) = (0,0). The counts are accumulated by the Quad counter and the EC727 MCSSCAs and are displayed on a formatted screen and in the data file. The information is written in 2 records : - Record A contains the coordinate and the 4 QCR counts while record B has the counts from the six SCAs accumulated by the EC727 module. During data collection, the four QCR values are continually displayed for information. The X motor is then moved to coordinate (1,0) which may be a positive or negative step in the motor. Negative step scans will be slower due to backlash correction. Collection in increasing X is completed as above until nsteps in X have been achieved. Next the Y motor is incremented by Ystep and the X-stage is driven back to the Xstart and the X-motor is scanned through as before. This continues until all X,Y coordinates as specified by the scan parameters have been covered. Motors will remain at their final positions at the end of the scan.

READ_DETECTORS Synonyms R RE REA READ

This option monitors the counts accumulating in the Quad Counting Register channels 1-3 (channel 0 controls the timing period). After the specified period has elapsed, all channels are displayed on the screen.

The user is prompted for a count time in Secs (default 1 sec)

QUIT Synonyms Q QU QUI QUIT

Use this command to leave the program. It will bring you back to RT-11 command level.

3.4 TFILE

This program is used to transfer datasets from the station computer to larger computers for permanent storage and data analysis. All data must be transfered to the convex for permanent storage, although most data analysis is carried out on Vax A (DLVA). It is recommended that all data sets are transfered to the convex and then copied to the Vax when you are ready to analyse the data. After a dataset is transfered to the convex the filename on the station computer is changed from Rxxxxx.DAT to Rxxxxx.CON, where xxxxx is the run number. Only ever delete .CON files from the station computer and remember to transfer all data files to the convex before you leave.

4 Standard 9.7 file formats

The data acquisition programs available on station 9.7 produce data files with various formats as summarised in table (3). There are two standard file formats at the **SRS**: OTOKO format and SRS format, the former is binary the latter ASCII.

4.1 SRS MCA Data

Whenever the word SRS appears in the name of an output datafile, it specifies that the file is in ASCII format and has a standard header. This header consists of a number of parameters in a Namelist format which is recognised by a number of data analysis programs on site. It also is used during NAS/Convex data archiving. The first records of a dataset are as follows :

```
&SRS
SRSRUN=12950,SRSDAT=800729,SRSTIM=151042,
SRSSTN='INT9',SRSPRJ='XXXXXXXX',SRSEXP='XXXXXXXX',
SRSTLE='BA GAMMA SOURCE                                                ',
SRSCN1='        ',SRSCN2='        ',SRSCN3='        ',
&END
&PARAMS
PARM( 1)=   237.03    ,PARM( 2)=  0.00000    ,PARM( 3)=  0.00000    ,
&END
 Accumulation Time for Data =    417 Seconds
 Temperature from Chart Recorder (Volts) 0.02
    626.     452.     453.     464.     441.     419.     433.     448.
```

The standard SRS namelist is contained between the &SRS and &END delimitors. Within this block, the SRSRUN parameter shows the runnumber of the raw file as specified on the station i.e. the above file would have been saved as R12950.DAT. The date is saved at the time of creating the file i.e. 29th July 1980 in this case. The time in SRSTIM is shown in HHMMSS format. Other parameters will have been prompted for by the data acquisition program being a title string of 60 characters (SRSTLE), and 3 user defined parameters (SRSCN1-3) each of 8 characters. Records following the SRS namelist may vary with future revisions of software.

In addition to the standard namelist parameters, user parameters may be appended to the header as a parameters namelist. In the case of DEDS, the input counts from channels 1 to 3 of the Quad Counting registers are written for the last MCA data collection period in question, as a parameters namelist (NB Quad counting channel 0 is reserved for program timing). This is indicated by the &PARAMS delimitor.

After the namelist, it is possible to add comment records providing that an alpha character (A-Z) appears in the 1st 4 columns of the record. In DEDS, the total accumulation time for the data is written in this way which may be the result of data collected over several discrete collection periods (see PROCESS option). In some instances, user comments can be added which are preceded by the "COMM " statement.

Following the header information, the data is written. It is written with Fortran 1X,8F9.0 Format. There may be 4000 or 2000 channels of MCA data depending on the program mode. If 4000 channels is specified, the SRS data files will occupy 38Kbytes of diskspace.

4.2 SRS Column Data

This data always has the standard SRS header (see SRS MCA Data) at the start of the file. After various comments and program-specific information, the data will appear in column format. This usually represents one or more continuously varying X columns, e.g.motor positions, and the resulting Y data e.g. 4 input channels of a quad counting register (QCR). With the Tomography scan in TOMO, there is a motor (X,Y) coordinate followed by the 4 QCR inputs and 6 single channel analyser (SCA) inputs to save. This requires the unusual step of writing the SCA data on the next record in the file. This may cause probems with sandard analysis programs which expect identical data records rather than repeated pairs.

4.3 Temporary Column data

The TOMO program produces a temporary data file that is exactly the same as the SRS column data except that there is no namelist at the start of the file. This data is accepted by standard data analysis programs but cannot be archived on the Convex.

In the case of the TOP program suite, data when in column format is generally saved initially as a temporary column data file which is not available to the user. On specifying to SAVE the data, it can be saved either to a user-specified column dataset, or a standard SRS file. If neither of these options is chosen, the data will be overwritten during the following scan. The TOP SWEEP scan is not of this form as it produces binary data (see OTOKO Binary Data).

4.4 OTOKO Binary Data

OTOKO files are in three parts a header file, a data file and a calibration file. This file format is used by the non-crystalline diffraction project team at the SRS, and is named after their data analysis package OTOKO.

4.4.1 File naming convention

The header file is in ASCII and contains information such as the title, file names, start and end time of scan, file size and scan conditions. It has the generic name xxx002.MDD.

The data file is a direct access binary file, written by a statement of the type WRITE(IOUT'IREC) (DATA(k),k=1,NCHAN), and contains 4-byte floating point values representing the signal count rate. Each record corresponds to a complete spectrum of 1-d sweep. It has the generic name xxx002.MDD.

The calibration file is of the same format as the data file but contains the monitor spectrum or reference count rate. It has the generic name xxx002.MDD.

The naming convention is as follows: xxx represents a run number from A00 to Z99. 000, 001 and 002 stand for header, data and calibration file. MDD stands for Month and date: 119 for january 19th and C31 for december 31st.

So, files A89000.123, A89001.123 and A89002.123 are the header, data and calibration files of run A89 produced on the 23rd of january.

4.4.2 Formatting conventions

The HEADER file format is as follows:

First record 80-character title containing date and time.

Second record 80-character title containing a comment.

Third record 10 integers in I8 format with the following significance:

1 The number of data points in each record.

2 The number of records in the dataset.

3 The number of datasets in the same DATA/CALIBRATION file.

4 The data type.

0 REAL*4 (The only one supported at present)

5-9 Spare

10 Indicates presence of calibration data file:

0 no calibration data

1 associated calibration data file

The data values themselves are written in the data or calibration files opened as direct access files by Fortran unformatted write statements.

Fourth Record the name of the DATA file (14A1) followed by the global minmax values (11X,G15.5,11X,G15.5)

Fifth Record Same as third but refers to calibration file attributes.

Sixth Record the name of the CALIBRATION file (14A1) followed by the minmax values (11X,G15.5,11X,G15.5)

If the third number of the third record is greater than unity it indicates that another set of records as for record 1 to 5 is expected for corresponding information on subsequent datasets in the same data calibration files.

Given below is an example of a HEADER file produced by the DEDS program in 4000 channel binary mode (PROCES then SAVE options):

```
SRS DATA RECORDED ON 14-JUN-88 AT 13:05:43
JUNK.DATA
    4000       1       1       0       0       0       0       0       0
B22001.614    . MINIMUM :     0.00000     MAXIMUM:     0.16000E+08
```



```
-----------------------------------------------------------------
Data collection time     10 Secs
13:05:43           10.       0.        0.        ·0.
```

In this instance, only a data file exists (no calibration file). It contains 1 record in total consisting of 4000 REAL*4 binary MCA channel values.

In the AUTOSCAN option of DEDS, two MCA spectra are collected at once and so the OTOKO files include a calibration file with data in the same format as that of the data file. Both are described by a single header file.

Lines after the data and calibration file names are ignored by OTOKO/BSL because the SET index is 0 (3rd number in 3rd record). The additional timing and QCR values have been written as comments by DEDS. This section of the header will vary depending on the program which has produced it.

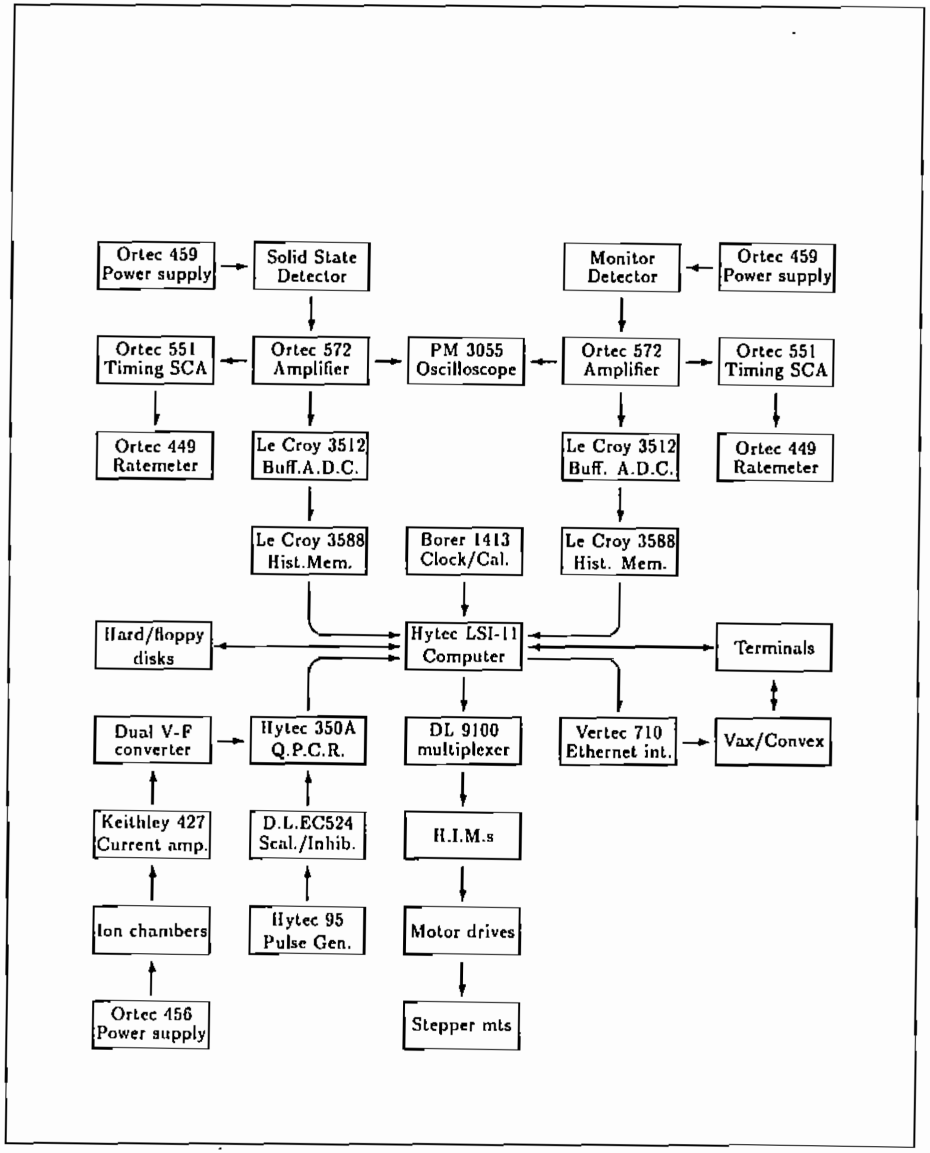

Figure 1: Block diagram of station electronics

1	NE 9100 multiplexer (1)
2	NE 9100 multiplexer (2)
3	VTC 710 Ethernet board
4	BORER Clock/Calender
5	EC 728 Time frame generater
6	EC 727 Multichannel scaler
7	Hytec 95 Pulse generater
8	EC 524 Scaler inhibitor
9	Hytec 350A Quad counter (1)
10	Hytec 350A Quad counter (2)
11	LeCroy 3588 Histogramming memory (1)
12	
13	LeCroy 3512 ADC (1)
14	
15	
16	LeCroy 3588 Histogramming memory (2)
17	
18	LeCroy 3512 ADC (2)
19	
20	
21	
22	EC 608 Module to module controler
23	
24	Sension 1536 Crate controller
25	

Figure 2: Schematic diagram of CAMAC crate

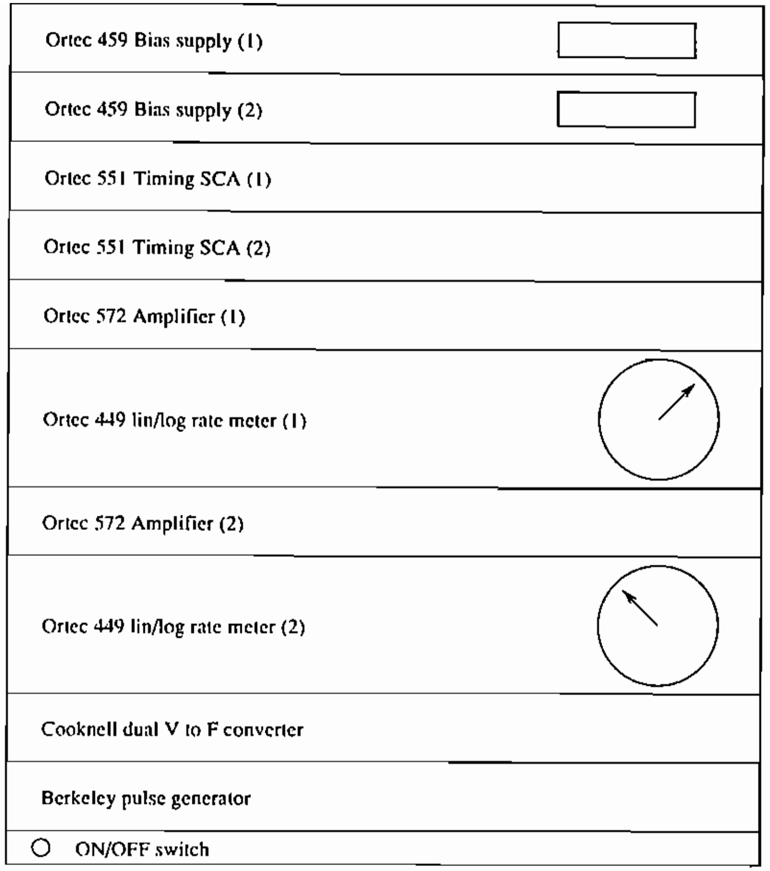

Figure 3: Schematic diagram of NIM crate

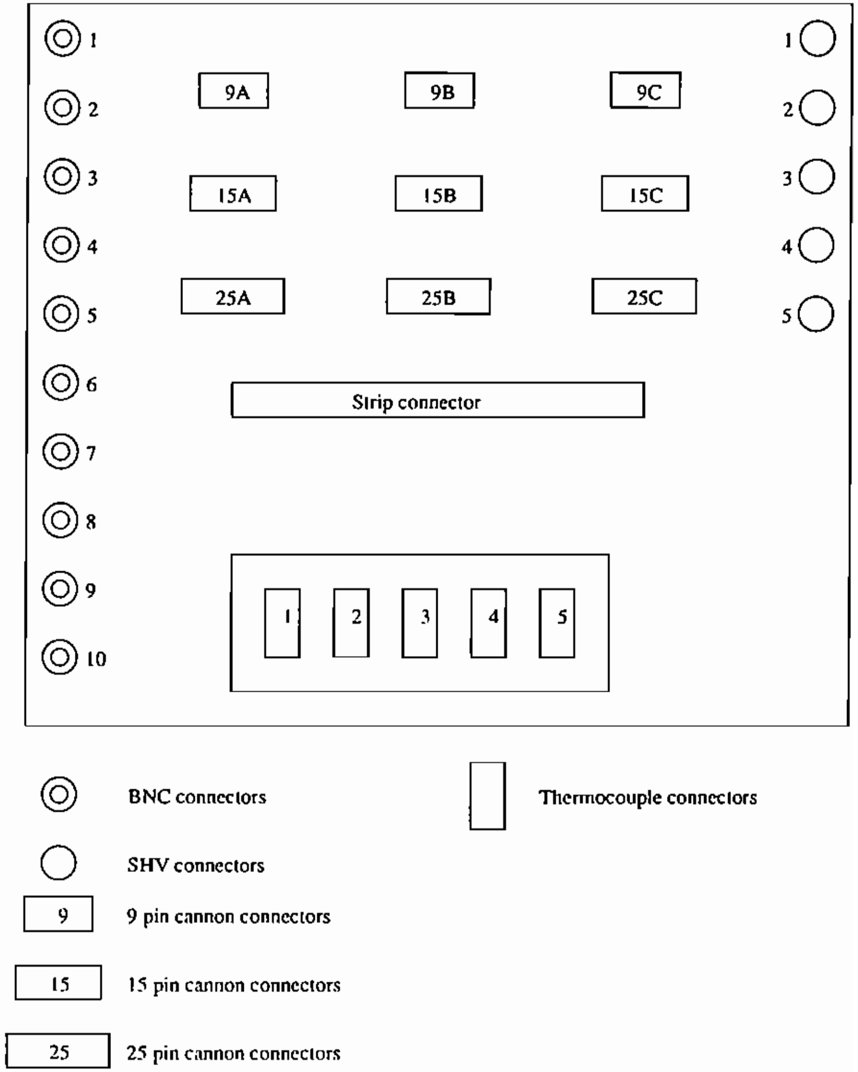

Figure 4: Schematic diagram of interface box

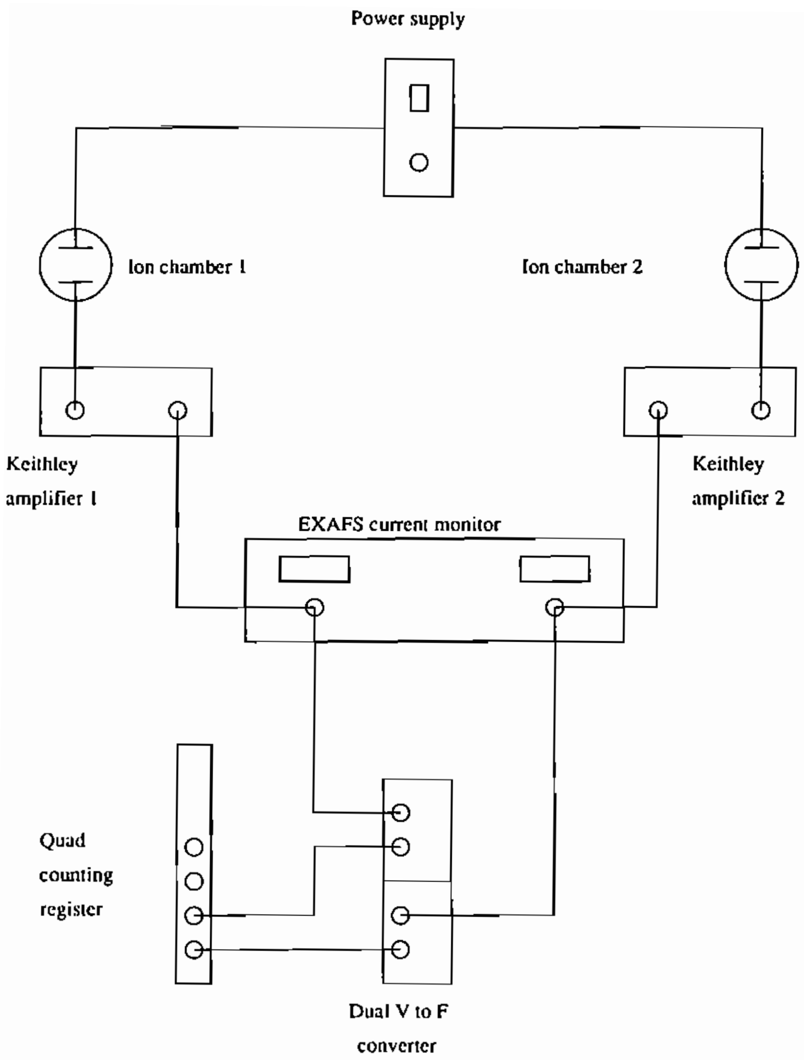

Figure 5: Schematic diagram of ion chamber electronics

HIM	Cable number	Motor driver	Motor type	Polarity	Use
1	10	CD 30	3-6 A/P	Bipolar	X-axis
2	13	CD 30	3-6 A/P	Bipolar	Y-axis
3	8	CD 20	2-3 A/P	Bipolar	
4	15	CD 20	2-3 A/P	Bipolar	Pinhole
5	5	CD 20	2-3 A/P	Bipolar	
6	11	CD 20	2-3 A/P	Bipolar	
7	12	CD 30	3-6 A/P	Bipolar	Z-axis
8	14	CD 30	3-6 A/P	Bipolar	
9	16	TM162C	0-2 A/P	Unipolar	HS1 or X-arc
10	17	TM162C	0-2 A/P	Unipolar	HS2 or Y-arc
11	18	TM162C	0-2 A/P	Unipolar	HS3
12	19	TM162C	0-2 A/P	Unipolar	HS4
13	20	TM162C	0-2 A/P	Unipolar	
14		CD 20	2-3 A/P	Bipolar	
15		CD 20	2-3 A/P	Bipolar	
16					
17	1	LD 2	900 mA	Unipolar	TC1
18	2	LD 2	900 mA	Unipolar	TC2
19	3	LD 2	900 mA	Unipolar	TC3
20	4	LD 2	900 mA	Unipolar	TC4

Table 1: Arrangement of stepper motor drivers on station 9.7

Key	Title	Function
1	TC1	Move extra beam definition slit
2	TC2	Move extra beam definition slit
3	TC3	Move front verticle divergence slit
4	TC4	Move back verticle divergence slit
5		
6	XTRANS	Move motion parallel to X axis
7	YTRANS	Move motion parallel to Z axis
8	ZTRANS	Move motion parallel to Z axis
9		
A	XARC	Move arc parallel to X axis
B	YARC	Move arc parallel to Y axis
C		
D	HS-Y	Move Huber Slit marked A
E	HS+Y	Move Huber Slit marked B
F	HS-Z	Move Huber Slit marked C
G	HS+Z	Move Huber Slit marked D
H		
I	PINHOLE	Move beam defining pinhole
J		

Table 2: Motor keys used in the powder diffraction MOVE menu

File Type	Program
SRS MCA Data	DEDS
SRS Column Data	TOMO, TOP
Temporary Column data	TOMO, TOP
OTOKO binary Data	DEDS, TOP

Table 3: Relationship between data acquisition programs and file types