



Technical Report
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CRISP Instrument Manual

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May 1997

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CRISP Instrument Manual

David G Bucknall and Sean Langridge

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1. INTRODUCTION

CRISP is one of two neutron reflectometers at ISIS. It is the original instrument and designed to be a general purpose reflectometer for investigation of a wide spectrum of interfaces and surfaces. The sample geometry is horizontal and therefore a wide range of samples can be investigated from air-liquid, liquid-solid to solid-solid cases in all disciplines of science. The instrument uses the pulsed neutron beam obtained from ISIS neutron facility and viewing a hydrogen moderator gives a normal neutron wavelength range of 0.5 - 6.5 Å. A large variety of sample environment equipment is available to users. The instrument unlike its sister SURF can also be run in a polarised mode allowing polarised neutron reflectivity (PNR) measurements as well being able to perform full polarisation analysis PNR (PA-PNR). The CRISP instrument is highly automated allowing precision reproducible measurements.

1.1 Location of instrument

The CRISP neutron reflectometer is found on the north side of the ISIS Facility experimental hall (building R55), between the LOQ small angle scattering instrument and the SURF reflectometer. See Figure 1. The instrument blockhouse is found on the ground floor and shares a common entrance area with SURF, with the instrument control cabin on the mezzanine level, immediately above the blockhouse.

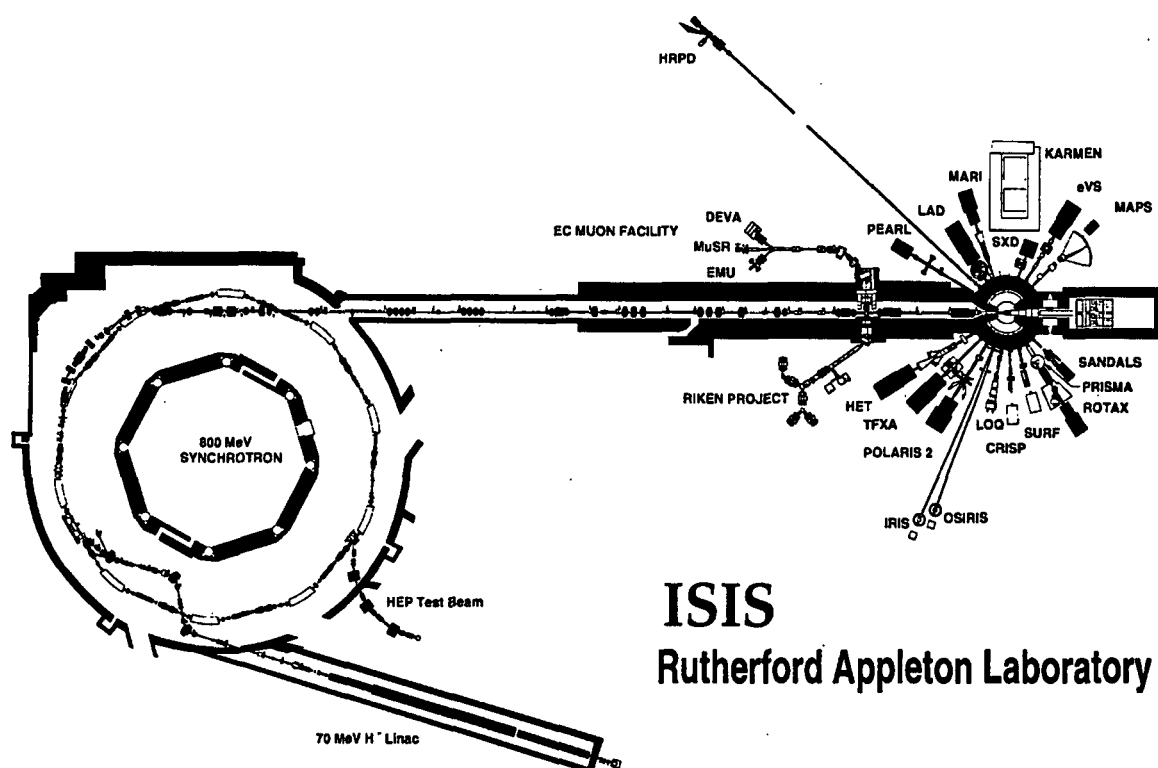


Figure 1: Schematic diagram of the ISIS experimental hall, showing the position of the CRISP instrument.

1.2 Instrument scientists

The following are the instrument scientists who work on the CRISP instrument. The extension numbers apply to on-site telephones. If phoning from outside site then the full number is +[44] (0) 1235 44 +☎. Bleeps can be operated by dialling 70- 1- 🔔- ☎# (where 🔔 is the bleep number you require and ☎# is your extension number followed by a #). After dialling 70 all the instructions are given.

		☎	🔔
CRISP Instrument responsible:	David Bucknall	6437	273
Instrument scientists	Sean Langridge	5269	280
	Jeff Penfold	5681	187
	John Webster	6381	201

1.3 Safety in the Experimental Hall

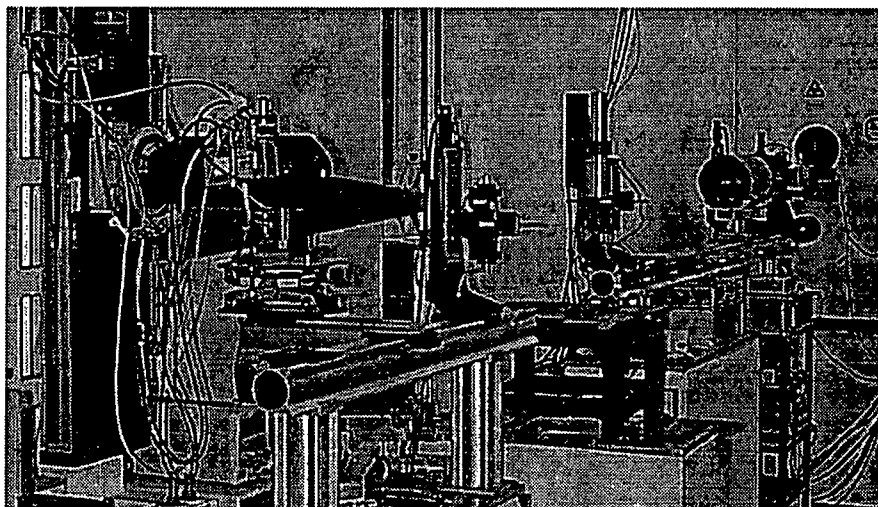
There are many things to remember when within the experimental hall in order to work safely. Many of these are the same safe practices used in any laboratory, but the presence of radiation means that we have several extra procedures which must be followed. On entering the experimental hall for the first time, it is *essential* that every new user watches the safety video. Two video units can be found on site, one in building R3 and the other in the common area on the north side of the hall (where the vending machines can be located). Every user should sign the supplied cards to indicate they have watched the video. In addition, a safety package including all relevant information will be distributed to new users.

As part of the safety system, entrance to the experimental area is via swipe card doors. Every member of the experimental team must swipe their individual cards. Cards for this swipe card system must be obtained on arriving at RAL during registration. At the same time a radiation badge must also be collected and worn in a prominent position on your person at all times you are in the experimental hall.

If there are any questions regarding any aspect of safety please contact your local contact in the first instance or the Main Control room on extension 6789.

		☎
Useful telephone numbers:	Main control room	6789
	Health physics (monitoring)	6696
	Emergency (fire, ambulance)	2222
	Occupational Health	6666

2. THE CRISP NEUTRON REFLECTOMETER



The essence of a neutron reflection experiment is to measure the specular reflection as a function of the wave vector transfer, Q , perpendicular to the reflecting surface. This can be related to the neutron refractive index profile normal to the surface and interface, and is often simply related to the scattering length density. This yields information about the composition and density gradients at surfaces and interfaces.

The CRISP instrument neutron reflectometer uses a broad band neutron time-of-flight (TOF) method for determining the wavelength, λ (and hence Q), at fixed angles, θ . A schematic layer out of the instrument is shown in Figure 2. Much of the instrument is highly automated allowing precision control and high degree of reproducibility.

The instrument views the 20K hydrogen moderator giving it an effective wavelength range of 0.5-6.5 Å at the source frequency of 50 Hz extending upto a maximum of 13 Å if operated at 25 Hz. The incident beam is well collimated by both coarse and adjustable fine collimating slits to give variable beam size and angular divergence, with typical dimensions of 40 mm wide (horizontal direction) and anything upto 10 mm in height (vertical direction). A variable aperture disc chopper defines the wavelength band, and prompt pulse suppression is achieved by a nimonic chopper. Additional frame overlap suppression is provided by the nickel coated silicon wafer frame overlap mirrors, which reflect out of the main beam wavelengths greater than 13 Å. The instrument has two types of detectors, a ^3He single detector and a 1-D position sensitive multidetector.

The experimental arrangement is extremely flexible with the neutron beam inclined at 1.5° to the horizontal, which provides easy study of liquid surfaces. For liquid surfaces angles less than 1.5° are achieved by insertion of a supermirror. The sample position is designed to be vibrationally isolated from the rest of the instrument and further aided by active anti-vibrational damping. Solid films and solid-liquid

samples can be studied with ease, by use of a 2 arc, height adjustable sample position.

The CRISP reflectometer can easily be converted to a polarised neutron mode for the study of magnetic systems. This involves in the simplest case the use of a polarising mirror in a static field, a spin flipper and a static guide field. The sample is positioned either directly onto a goniometer or in an 4 position orange cryostat both of which can be mounted in one of two electromagnets. Full polarisation analysis is possible by inclusion of a post sample set of polarising mirror and spin flipper.

A summary of the instrument is shown below:

Incident Wavelength	0.5-6.5 Å at 50 Hz (0.5-13.0 Å at 25 Hz)
Optimal Q range	0.005 - 1.1 Å ⁻¹
Moderator	20K H ₂
Maximum beam size	40mm (H) × 10mm (V)
Detectors	³ He single detector (SD) & position sensitive multidetector (MD)
Data acquisition	VAX 3200
Moderator-sample distance	10.25 m
Sample-Detector distance	1.87 m
Choppers	Variable aperture disc chopper Nimonic chopper

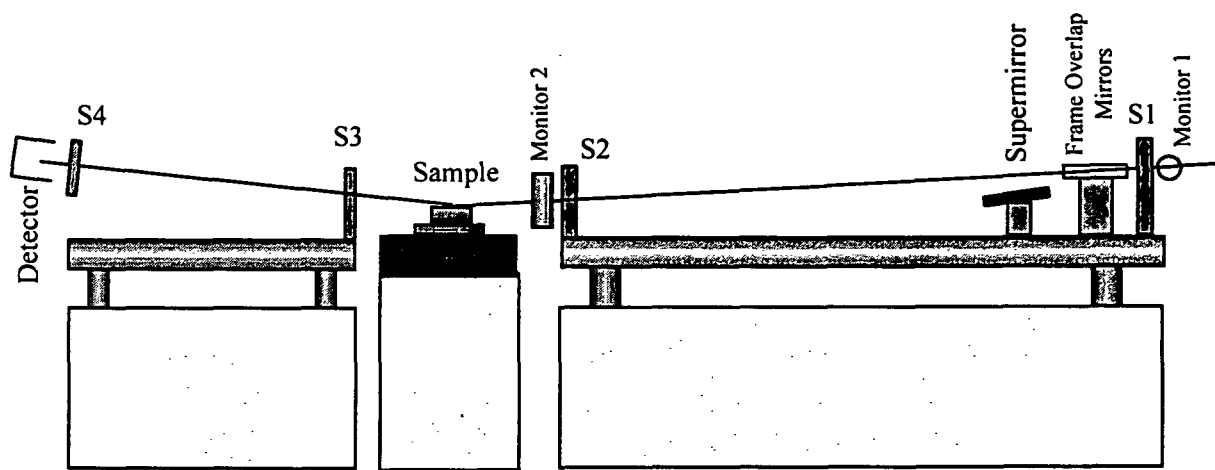


Figure 2: Schematic diagram of the CRISP reflectometer in non-polarised operation mode.

Most of the sample environment equipment and beamline components are controlled via a PC based system operating Micro-control motions. A typical display for is shown in Figure 3 for normal operation modes.

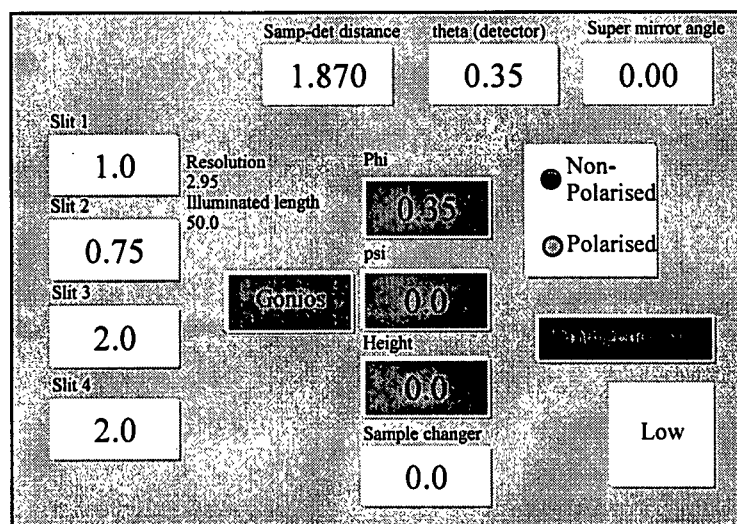


Figure 3: Typical Micro-control PC control screen display for non-polarised mode of operation.

Movement of any motion is achieved either manually by clicking on the box and inputting in the required value into the pop-up dialogue box or by command input from the VAX computer (see Section 3.2).

Polarised Neutron Reflectivity (PNR) mode

To perform polarised neutron reflectivity measurements the reflectometer can be easily re-configured to give a polarised incident neutron beam and, if required, full polarisation analysis of the outgoing neutrons.

Converting to polarised operation

Assuming that the reflectometer is in the non-polarised mode then the PC control panel should be "checked" in the non-polarised option and the super mirror angle set to zero. (When set to zero the super mirror/polariser is translated out of the incident neutron beam.) Clicking the polarised option should move the polariser in to the beam. Set the 'supermirror angle' axis to 0.35° (See Figure 4), this reduces the wavelength range to 2-6.5 Å.

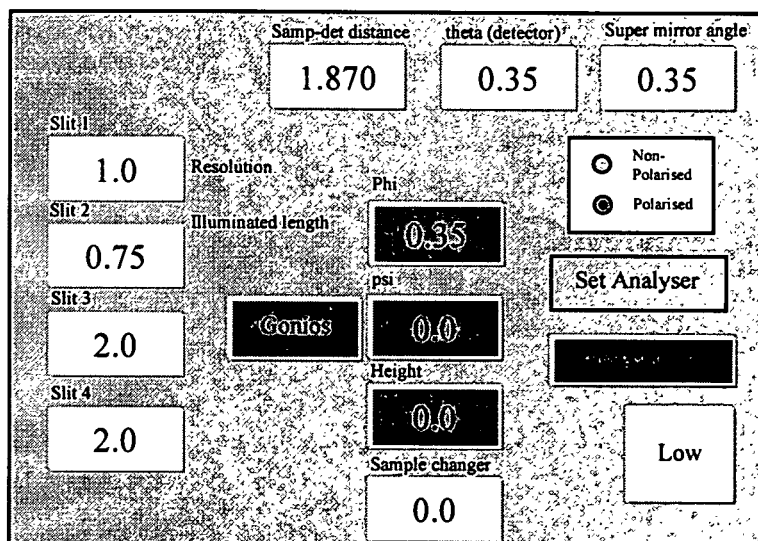


Figure 4: The reflectometer control panel in polarised mode

A schematic of the experimental set-up is shown in Figure 5 for full polarisation analysis. (For no polarisation analysis the second spin flipper and polarising mirror SF2 and PM2 are removed). Your local contact will install the sample environment options you require (magnet, cryostat *etc.*), the guide fields and the analysis kit. The polarising mirror (PM1) and the spin flipper (SF1) are permanently installed but may be translated out of the beam in the case of PM1.

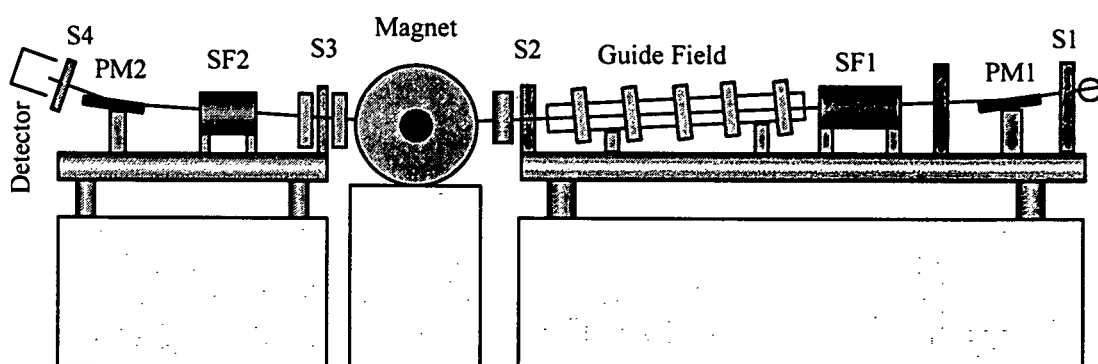


Figure 5: A schematic illustration of CRISP in full polarisation analysis (PA) PNR mode.

Before taking data there are several checks to be made to ensure that the polariser and spin flipper are correctly set-up:

1. Horizontal slits at PM1 and S2 are 20mm.
2. Given the finite length of PM1 the maximum vertical slit size for S1 is 1mm.

3. Guide field is in the same direction as the field at the sample position.
4. The power supply to SF1 (and SF2 if installed) are switched on and indicate ~1.5A.
Do not adjust these supplies.
5. Run the command file `pol_test` or `pol_test_pa` (PA-PNR) and verify that the power supplies are switching polarity every 15s.
6. Verify with your local contact that the CAMAC/DAE is set-up for multi-period data acquisition.

2.1 Sample Environment Equipment

The CRISP instrument has a standard set of sample environment equipment. Most of these are common to both reflectometers except the polarised neutron equipment which are only available to the CRISP instrument. Most of these have been built in house or been bought specifically for the use on the beam lines. In addition, a number of special pieces of equipment built by university teams have also been used. A brief summary of the key pieces of sample environment equipment is given below, users should contact David Bucknall or their local contact if they are unsure which is most applicable to their experiment. In some circumstances especially with new types of experiments special equipment may have to be developed which should be done in close association with the CRISP instrument scientists.

2.1.1 Standard Goniometer Configuration

The standard normal reflection mode of the reflectometer has a 2 arc goniometer stack (ϕ and ψ motions) on top of a linear translation stage which is all mounted on a height table. The motions except the height table are standard Micro-controlle equipment. Drawings of the layout of the sample area configuration is shown in Figure 6. For liquid samples the goniometer stack is removed and an active anti-vibration table fitted.

The key parameters and load capacities of the sample position is listed below:

Motion	Range	Resolution	Load capacity
BG80 (ϕ motion)	$\pm 45^\circ$	0.001°	12 kg
BG120 (ψ motion)	$\pm 45^\circ$	0.001°	20 kg
Linear translator	600 mm	<0.05mm	120 kg
Height table	100 mm	<0.05mm	100 kg‡
Anti-vibration table	----	----	150 kg

‡ This is on top of the standard environment equipment.

The minimum distance from height table surface to beam centre is 236 mm and the maximum is 341 mm. If the translator is added these figures are modified to 121 mm (min) to 226 mm (max).

Sample mounting on the goniometer is via a kinematic plate. If users wish their equipment to fit onto these plates then they should contact David Bucknall for full design drawings.

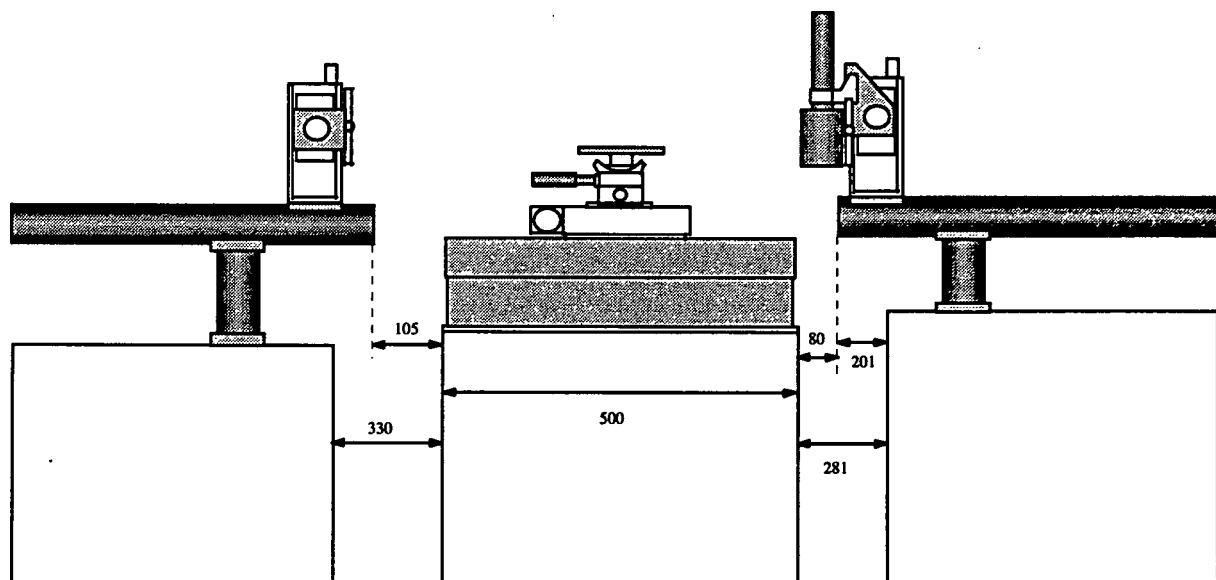


Figure 6: Plan and elevation picture of the CRISP sample position showing table and goniometer stack on top of the translator (see also drawings in Appendix).

2.1.2 Liquid troughs

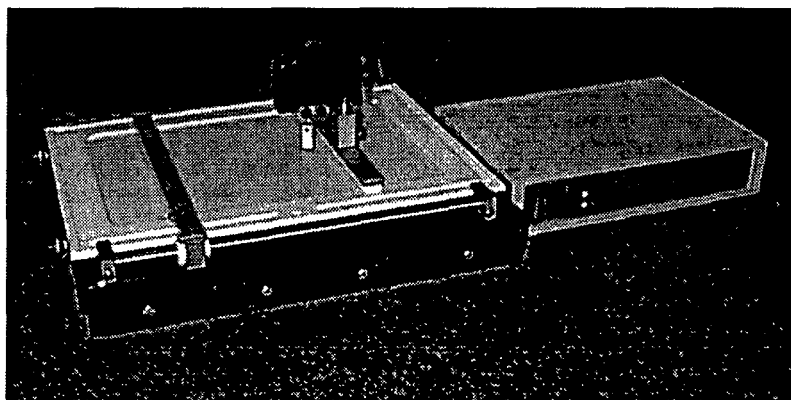
The multi-sample liquid troughs has the capacity for 4 liquid samples in individually sealed containers. Each unit contains a PTFE trough and is heated via heating mats. The units have the capability to be sealed to prevent evaporation of even volatile samples. Almost all of the construction is made from aluminium with quartz windows to allow laser alignment of the samples. All four units are also held within a temperature controlled box to reduce condensation effects. The whole unit mounts directly onto the active anti-vibration table which is itself mounted to the linear translator. This allows the possibility of measuring all four positions remotely under computer control.

The summary of the liquid troughs is given below:

Cell temperature range	RT - 80 C
Outer unit temperature range	RT - 80 C
Sample volume (approx)	70 ml

The sample volume is assuming use of a water subphase which gives a good meniscus which is a few millimetres higher than the lip of the PTFE trough.

2.1.3 Nima Langmuir Troughs



There are two Nima Langmuir troughs available for use on CRISP and SURF. Both have double moveable barriers allowing the measurement of reflectivity curves *in-situ* over a very wide area enclosed by the barriers. Both troughs are computer controlled with a user friendly interface allowing flexibility of use. A majority of experiments will need to be carried out holding a fixed pressure over the length of the reflectivity measurement and this can easily be achieved as well as measuring more normal pressure-area curves. Full details of the use of the troughs can be found in the very helpful Nima handbook. The large Nima trough has moveable fixed barriers which allow the volume of subphase to be varied. The troughs both have perspex lids which incorporate neutron transparent quartz windows. This arrangement allows easy alignment of the liquid but prevents a majority of the airborne dust contaminants. This is not however a sealed unit and is therefore not vapour pressure tight. The troughs both have the possibility to link to a recirculating heater/cooling bath which has a maximum temperature range of -50 - 200 C. However, temperatures above 100 C are not recommended for the PTFE.

Care must be taken to ensure that the troughs are set up correctly and it is advised that users contact David Bucknall before using the equipment. Calibration of the area enclosed by the barriers will be done before users will have access to the troughs although calibration of the pressure head will be the responsibility of the individual users. Again contact David Bucknall if there are any problems.

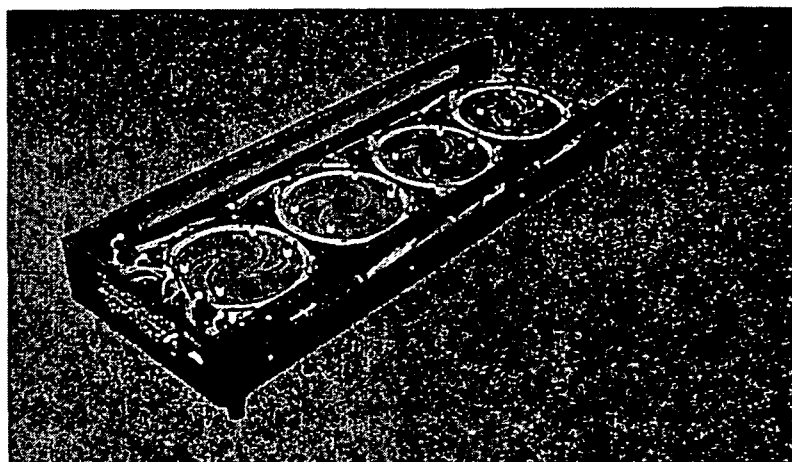
A summary of the key features of the Nima troughs follows:

Small Nima Trough

Internal dimensions	200 × mm
Average area coverage	90 - 540 cm ²
Typical subphase volume	300 cm ³
Temperature range	-50 - 100 C

Large Nima Trough

Internal dimensions	200 × mm
Average area coverage	90 - 1080 cm ²
Typical subphase volume	upto 1500 cm ³
Temperature range	-50 - 100 C

2.1.4 Solid Sample Changer

The four position sample holder mounts directly onto the standard goniometer stack will take samples which are typically silicon or quartz substrates, ranging from 10 to 100 mm diameter. Two modes of operation can be achieved by changing the sample holding inserts. One insert allows for 4 independent temperatures on the 4 sample positions via heater cartridges giving temperature from RT to 350 C. The other insert is temperature controlled by connection to a recirculating bath giving a temperature range from -50 - 200 C. This cannot be achieved by each sample independently since the circulating fluid runs underneath all the samples. The samples are housed in a metal box with quartz windows allowing for laser alignment with a perspex lid. The unit is not sealable but allows for inert gas to be passed through it under a positive pressure (the unit does not allow the samples to be placed under vacuum).

Summary of the equipment:

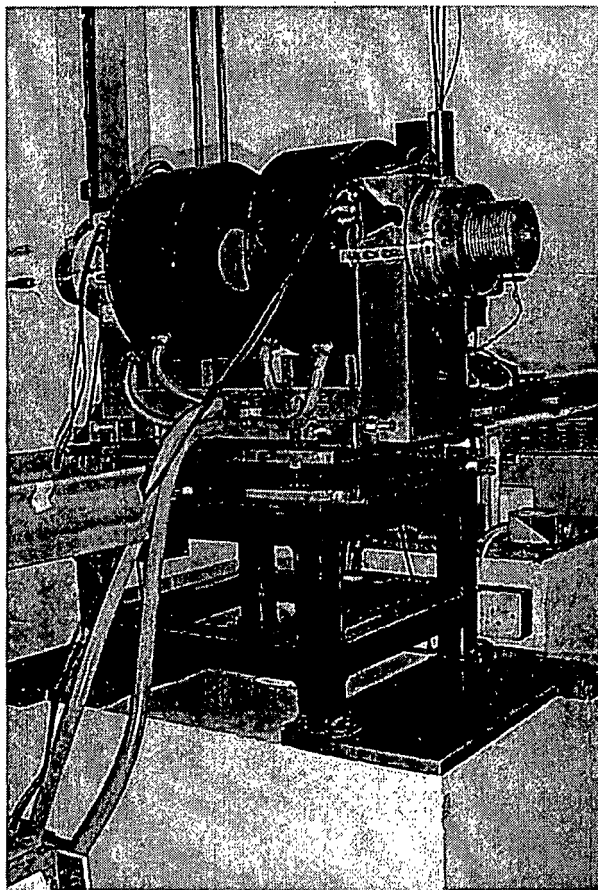
Heated Insert

Number of samples	4
Independent sample heating	yes
Sample size	10 - 100 mm diameter
Temperature range	RT - 350C

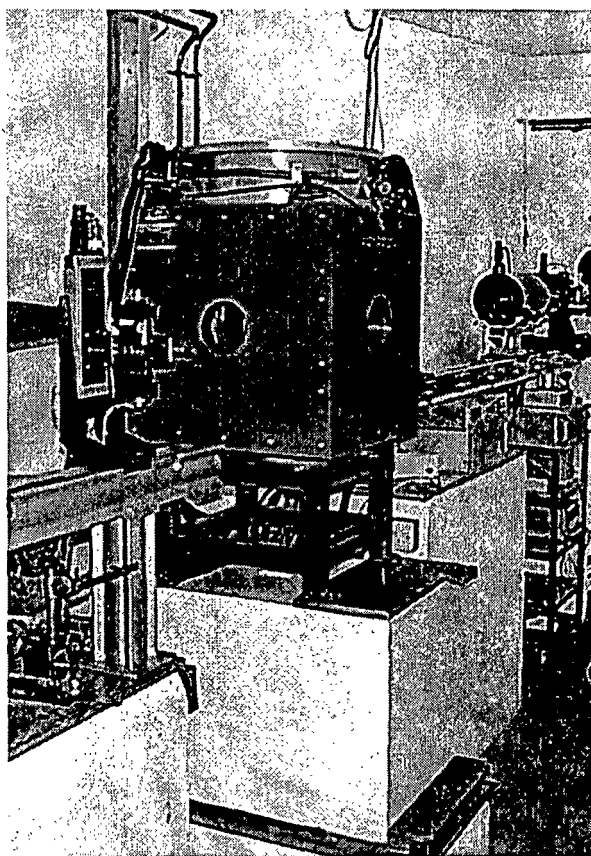
Heated/Cooled Insert

Number of samples	4
Independent sample heating	no
Sample size	10 - 100 mm diameter
Temperature range	-50 - 200 C

2.1.5 Newport/Goudsmit Electro-Magnets



Newport Magnet



Goudsmit Magnet

The sample stage accepts two water cooled electro-magnets which can be used to provide a continuous magnetic flux density up to 1.5T. Both magnets have the capability to hold an "Orange ILL" type cryostat (see section 2.1.6). The main characteristics of the two magnets are detailed in table below.

Magnet type	Max field at 20mm gap	90mm gap	Field direction*
Newport	1.0 T	0.5 T	Longitudinal
Goudsmit	---	1.6 T	Longitudinal and transverse

*Relative to the neutron beam direction

Currently only the Newport magnet is commissioned on CRISP. The Goudsmit magnet should be available before the end of 1997. As the installation of both magnets is a complicated process and should not be undertaken by external users. If requested on the application form the magnet will be installed by your local contact at the beginning of the experimental run. Please discuss your magnetic field requirements with your local contact in advance of any experiment.

Measuring the magnetic field

A "Hirst" teslameter is available in the CRISP cabin to measure the magnetic field strength of the magnet and the neutron guide fields. The hand held unit is simple to operate although care should be taken to ensure the correct Hall probe is used to measure either the longitudinal or transverse magnetic field.

Safety and the Newport magnet

The Newport magnet will be installed at the beginning of your experiment by the local contact but there are several safety issues which you should be familiar with before operating the magnet:

- The presence of an *input* voltage to the power supply is indicated by the "Magnet On" sign in the blockhouse. If illuminated then there is the possibility that the magnet is energised and users must ascertain if the magnet is actually powered (measure the field or check the power supply).
- The power supply can be immediately shut off by tripping the interrupter switch which is clearly marked on the CRISP blockhouse wall.
- The electrical connection for the magnet is located in the CRISP blockhouse. It is essential that if the magnet needs to be connected/disconnected then the power *must* be shut-off either at the power supply or by tripping the interrupter switch.
- Cooling water *must* flow through the magnet at all times, even at low operating currents.
- When energised care should be taken to avoid introducing magnetic materials (e.g. watches, screwdrivers) near to the pole pieces.

2.1.6 Cryostat

A specially adapted "Orange ILL" type Helium cryostat is available on CRISP to provide operating temperatures down to 1.4K. For temperatures below 4K a "Roots" vacuum pump set is provided. The RAL reports 93-006 and 92-041 describe the operation of the cryostat and we outline only the salient points here. At the beginning of the experimental run the prepared cryostat will be installed on the instrument by the user support group. Given the relative complexity of the cryostat it is essential that users should contact either their local contact or the sample environment group (see phone list in Section 6) if they are uncertain of any of the correct operational procedures for changing samples, cooling, warming etc.

The valves on the cryostat, in particular the cold valve, are very delicate and should only be closed finger-tight. Do not over-tighten these valves as serious damage may result.

Typical temperature ranges achievable by cryostat:

	Temperature range	Stability
Normal operation	$\geq 4\text{K}$	$\pm 0.1\text{K}$ (at 4K)
With Roots Pump	$\geq 1.5\text{K}$	$\pm 0.1\text{K}$ (at 1.5K)

The CRISP centre stick allows four samples to be mounted in the Orange cryostat with computer control of the height and angle axes. The maximum sample dimensions are: 29 × 30 mm.

3. RUNNING THE INSTRUMENT

3.1. Aligning samples

There are essentially two methods of sample alignment, either by laser or using neutrons. The laser beam travels along the same path as the neutrons. The choice of method depends on the sample. For solid films or liquids where the laser can be reflected off the sample then the use of the laser is preferable. If the use of complex sample environment is used where the laser can not transmit through the sample, then alignment may only be possible with neutrons.

3.1.1 Laser alignment

To start alignment of solid samples using the laser, the perpendicular goniometer motion (psi - ψ) must be adjusted so that the surface of the sample is perfectly horizontal. Then the following slit and detector arrangement is recommended:

Motion	Setting
S1	1.0 mm
S2	0.5 mm
S3	4.0 mm
S4	10.0 mm
THETA (θ - detector angle)	0.6°

1. Ensure that PHI (ϕ - sample angle) is non-zero with respect of the laser beam remembering that the beam is inclined at 1.5° to the horizontal.
2. Adjust HEIGHT so that the laser beam fully illuminates the sample surface and gives a maximum in the reflected beam intensity.
3. Adjust PHI until the laser beam equally illuminates the slit at the back of the single detector slit. (If using the multidetector then PHI should be adjusted until the laser beam hits the pencil mark indicated on the face of the detector).
4. Redefine PHI on the control PC. This is achieved by clicking on the GONIOS box on the screen and choosing either the 'Redefine PHI motion' box and type in the value of THETA (in this case 0.6) or clicking on 'PHI = THETA and HEIGHT = 0' box.

If using liquid surfaces (without the supermirror) the detector angle should be set to 1.5°. The slits are slightly different since the sample is larger and given below. Since no goniometer is used then the only adjustable motion is the height of the sample. This should be moved until the reflected laser beam sticks centrally on the detector slits.

Liquid Surface Parameters	Setting
S1	4.0 mm
S2	2.5 mm
S3	4.0 mm
S4	10.0 mm
THETA	1.5°

If using the magnet then these motions are achieved only using the manual goniometer adjustments. Your local contact will be able to demonstrate the use of this equipment. The cryostat has height and angle adjustments via a hand held remote control box. In both cases your local contact will be able to demonstrate the use of this equipment. However, the method of alignment is the same:

1. Ensure the sample is horizontal, orthogonal to the beam direction.
2. Adjust the ϕ angle of the goniometer so that the sample surface is approximately parallel to the laser beam.
3. Adjust the height of the sample so that the laser beam height is half its original value. This can be measured by placing a ruler in front of S3.
4. Iterate between 2 and 3 to give a sample half-cutting and parallel to the beam.
5. Set the detector to the angle of interest, e.g. 0.6° and adjust the ϕ angle so that the laser beam is aligned in the detector aperture and is symmetrically cut by slits S4.

Further iteration of the height and ϕ adjustments may be necessary to optimise the reflected intensity. It is worth noting that at small ϕ the height adjustment is well defined and conversely at large ϕ the alignment is relatively insensitive to the height but the ϕ angle is well defined.

Aligning the polarisation analyser

The polarisation analyser is mounted on a manual stage which can be installed on the post-sample section of the Micro-controlle X-beam. Alignment of the second polariser is made with an aligned sample and the reflected laser beam. In principle should you require PA-PNR then your local contact will ensure that the analyser is installed and aligned.

3.1.2 Neutronic alignment

The alignment by neutrons is essential for samples which are opaque to light such as solid-liquid cells. In these cases the instrument must be set up as indicated below. The sample will need adjusting so that PHI is defined and set to 0.0 and therefore parallel to the neutron beam. PSI may need adjusting to ensure that the sample is horizontal in the perpendicular direction. The HEIGHT should be moved so that the

laser beam strikes the cell slightly one side of the interface you are aligning on, ie the silicon - PTFE interface.

Neutronic alignment starting parameters	Setting
S1	1.0 mm
S2	0.5 mm
S3	2.0 mm
S4	2.0 mm
THETA	0.0°
PHI	0.0°

The sample is now ready for alignment and is achieved via a minimum of 3 alignment runs. A typical example set of alignments is given below:

1) Height alignment with $THETA = PHI = 0.0^\circ$

Defines the centre of the interface by finding the half height intensity from going from the neutron transparent silicon to the neutron opaque PTFE in this case.

2) PHI alignment at $THETA = 0.0^\circ$ and HEIGHT at half height

Determines the zero position of the PHI motion on a slightly coarse scale.

3) PHI alignment at $THETA = 0.25^\circ$

Determines the fine adjustment of the PHI motion.

These are performed using the program SCAN for each of these steps which should be run on the dashboard computer. SCAN asks whether the alignment scan is a height (adjusts HEIGHT motion) or a angle scan (adjusts PHI motion). Then the start value of the scan, step size, number of steps and number of microamps per step must be entered. Scans must be extensive enough so that the full range of the scan is achieved. The results of the SCAN program is performed within GENIE using the analysis program SCANNER, which requires information listed by the SCAN program after completion of the scan and displayed within the GENIE graphics.

A guide to parameters used for each of the scans is:

Scan	Motion	Start Value	Step size	No of steps
1) Height [PHI = THETA = 0.0]	HEIGHT	-1.0	0.1	21
2) Angle [THETA = 0.0, HEIGHT = ½ height]	PHI	-0.3	0.05	13
3) Angle [THETA = 0.25, HEIGHT = ½ height]	PHI	0.2	0.01	11

After each scan procedure the motions should be redefined using the GONIOS redefine click boxes. A typical session for in this case a height alignment is shown below:

```
CRISP> SCAN
Height (H), Angle (A) or Theta (T) scan ? H
Input starting height ==> -1.0
Input height step increment ==> 0.1
Input PHI angle of goniometer for scan ==> 0.0

load crisp$disk0:[crisp]height.upd

Input number of points in scan (less than 40) ==> 21
Input number of uamps per point (integer only) ==> 1
Are the slits and detector set up for a scan (Y/N) ? Y
```

at which point the command file is launched and the scan stated. After the scan has finished the run will be ended and stored and the following message will appear:

```
Scan start position   : -1.0
Scan step increment   : 0.1
Number of points      : 21

Please Analyse using SCANNER in Genie

load crisp$disk0:[crisp]normal.upd
CRISP>
```

The analysis is completed within GENIE running SCANNER, as the example shows below:

```
>> SCANNER
>> @USER$DISK:[DGB.GENIE]SCAN_ANAL
>>
-----
>>      SCANNER : Analysis of Axis scan for single detector
>>
>>                      DGB      24 Jan 95
>>
-----
>>
>>      Input scan run number ==>: 37700
>>      Input scan start value ==>: -1.0
>>      Input scan step increment ==>: 0.1
>>      Input number of points in scan ==>: 21
>>      Enter output workspace for scan (Wx) ==>: w10
>>
>>      ass 37700
>>      v5=0.1
>>      W1=S2
>>      .
>>      .
>>      .
>>      .
>>      load w10 sys$scratch:sum.out g:loader
>>      No. of points:      2
>>
>>      Error reading from transferred data file
>>
-----
```

```
>>      ascii file containing scan data is SYS$SCRATCH:SUM.OUT
>>
>>      at present in w10 (point mode)
>>
>>
>>
```

3.2 Dash Board Commands

A typical dash board display is shown below (see Figure 7). This screen is the control for the running of the instrument preventing beginning and ending runs from anywhere except this area. If for some reason the dash board is not present then it can be turned on with:

```
$CRISP> STAT ON
```

and conversely it can be turned off with:

```
$CRISP> STAT OFF
```

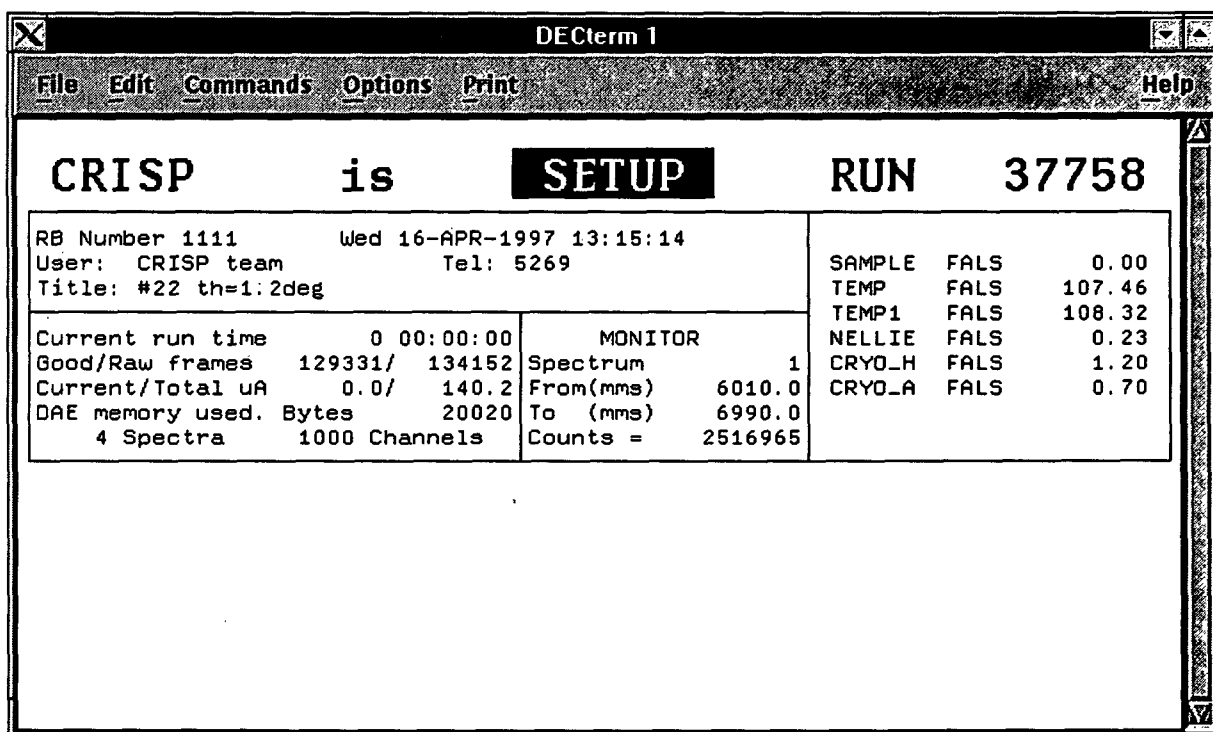


Figure 7: Typical dashboard display screen.

Commands for manual running of the instrument can only be submitted onto the dash board instrument control computer. Most commands are common to all ISIS

instrument although a number are specific to CRISP and SURF. A summary of the key commands are listed below.

Command	Description
BEGIN	Starts data collection, data is held in the DAE. The dash board will indicate RUNNING above the header block.
END	Ends the data collection and saves the data to file for archiving into a file CSP{run no}.RAW and therefore identifiable by the run number. The dash board run number will go into SETUP mode and increment the run number.
PAUSE	Pauses the data collection, the dash board will indicate a PAUSE mode.
RESUME	Resumes the data collection after the PAUSE statement has been issued and will return to the RUNNING mode.
ABORT	Ends the data run without saving the data. The DAE goes into SET-UP mode but the run number is not incremented.
SL	A command which must be used to move any of the Micro-controlle equipment. It should be given in the following format: SL {motion} {position} where {motion} is the motion to move and {position} is the value to move to. An example is: SL THETA 0.5 which moves the detector to 0.5°.
POL_RUN {X1} {X2}	A command file for normal PNR running which begins a run and counts for {Xi} frames on each spin state before switching to the other spin state. Typically X1=X2=5000 Since the command file does not contain any slit control information the beam line must be set up as required before running. This command file will continue until manually ended by {CTRL} Y followed by END or ABORT.
POL_RUN_PA2 {X1} {X2} {X3} {X4} @{file}	A version of the POL_RUN which runs the full polarisation analysis control. Typically X1=X2=X3=X4=5000 Runs a command file with the name FILE.COM which must be in the current directory. (See below)
UPDATE	Transfers the DAE data into the CRPT.
STORE	Writes the contents of the CRPT into a temporary file with a {run number}.SAV file extension

3.3 Writing command files

Command files are designed to allow multiple samples or angles (or both) to be run and therefore contain all the information required for changing slits, angles, and sample position. All the information for any automated control must be contained within the macro. The commands are duplicates of everything that can be input manually into the dash board computer. A typical file for looking at a sample at 2 angles is given below.

```
$ WSO:= WRITE SYS$OUTPUT
$ SL S1 0.48
$ WAIT 00:00:05
$ SL S2 0.22
$ WAIT 00:00:05
$ SL S3 2.0
$ WAIT 00:00:05
$ SL S4 2.0
$ WAIT 00:00:05
$ SL THETA 0.25
$ WAIT 00:00:05
$ SL PHI 0.25
$ WSO "Setting sample ANGLE to 0.25"
$ WAIT 00:00:05
$ CHANGE TITLE ""Sample at th=0.25deg""
$ BEGIN
$ WSO "CRISP Being Controlled by Command File"
$ WSO "AUTO.COM"
$ WSO "CONTROL Y To Exit - END or ABORT Run"
$ WSO "Waiting for 40 uAhrs before ending run"
$ WAITFOR 40 uamp
$ END
$ SL S1 1.148
$ WAIT 00:00:05
$ SL S2 0.524
$ WAIT 00:00:05
$ SL S3 3.0
$ WAIT 00:00:05
$ SL S4 3.0
$ WAIT 00:00:05
$ SL THETA 0.6
$ WAIT 00:00:05
$ SL PHI 0.6
$ WSO "Setting sample ANGLE to 0.6"
$ WAIT 00:00:05
$ CHANGE TITLE ""Sample at th 0.6deg""
$ BEGIN
$ WSO "CRISP Being Controlled by Command File"
$ WSO "AUTO.COM"
$ WSO "CONTROL Y To Exit - END or ABORT Run"
$ WSO "Waiting for 80 uAhrs before ending run"
$ WAITFOR 80 uamp
$ END
```

This command file is written in a normal DEC editor and must be saved with a .COM file extension. This example measures the reflectivity from the same sample at 2 different angles and adjusts the PHI and THETA motions as well as all the slits to enable the same illuminated length and resolution to be kept constant.

For samples that may require repeated runs then the following must be added before and after the section which needs repeating:

```

$ LOOP:
.
.
.
$ GOTO LOOP

```

3.4 Running in Polarised Neutron (PNR) Mode

3.4.1 Operating the Newport magnet power supply.

The Newport magnet is powered by a "Glassman LV series" dc power supply. The power supply is currently located on the ground floor near to the CRISP/Surf lab but will ultimately be located in the CRISP electronics cabin. The power supply can be run in both constant current and constant voltage modes. *The magnet requires constant current operation.* Having followed all the safety procedures outlined in the previous section and having familiarising yourself with the magnet/power supply set-up you are ready to operate the power supply:

- 1) Ensure that the standby button is depressed. *This cuts the output from the supply.*
- 2) Ensure that both the voltage and current controls are rotated fully counter-clockwise.
- 3) Check that the magnet is connected and that the cooling water is flowing.
- 4) Release the standby button. *This switches on the supply output.*
- 5) Slowly increase the voltage and current controls until the desired current is represented on the LED display and the supply is in constant current mode. (Current mode LED illuminated)
- 6) Before disconnecting the magnet slowly reduce the rotary controls to give zero readout on the two LED displays and place supply in standby mode. Switch off supply before disconnecting blockhouse plug.

It is essential that the magnet is not operated above 12A. This will cause excessive heating in the magnet and may ultimately damage the magnet or power supply. Additional information can be found in the Glassman power supply manual located in the CRISP cabin.

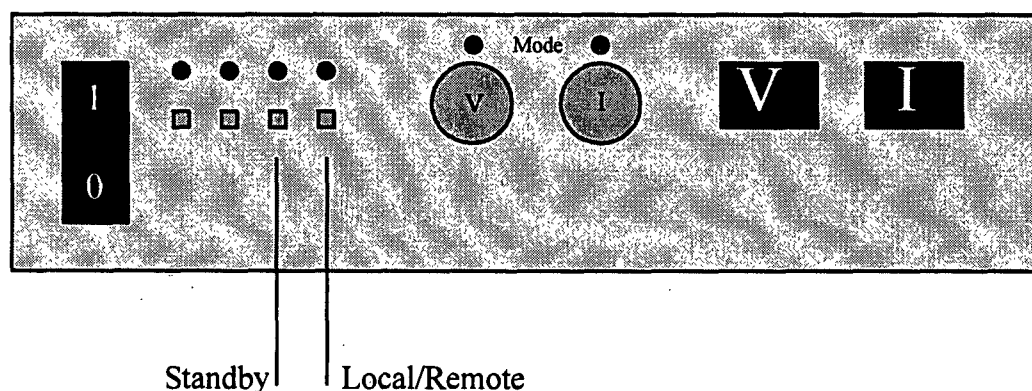


Figure 8: A simplified view of the Glassman Newport magnet power supply front panel

3.4.2 The Orange ILL Cryostat

- *Cooling to >4K.*

Open the cold valve half a turn and adjust the warm valve such that the Helium recovery flow meter indicates 10 l/min.

- *Cooling to <4K*

Close the warm valve, and open the cold valve 1/2 turn. Slowly open the Roots pump valve, never letting the pressure rise to above 10 torr. When the pump valve is fully open use the cold valve to set the flow to about 2 to 4 l/min.

- *Controlling at >4K.*

When the temperature is stable reduce the flow rate down to the value indicated on the information sheets accompanying the cryostat. Typically 2-6 l/min. To regulate the temperature above 4K you must use the "Eurotherm" temperature controller located in the CRISP electronics cabin. Before switching on the controller ensure that the heater is connected (at the cryostat) and that the output voltage is appropriate for the cryostat temperature. (At the rear of the rack is a multi-position switch for adjusting the output voltage) If in doubt start with the lowest voltage.

The cryostat temperature is indicated on the dashboard as TEMP and TEMP1 (see Figure 9). TEMP represents the cryostat temperature (labelled Cryostat-Fxd) whilst TEMP1 indicates the sample stick temperature.

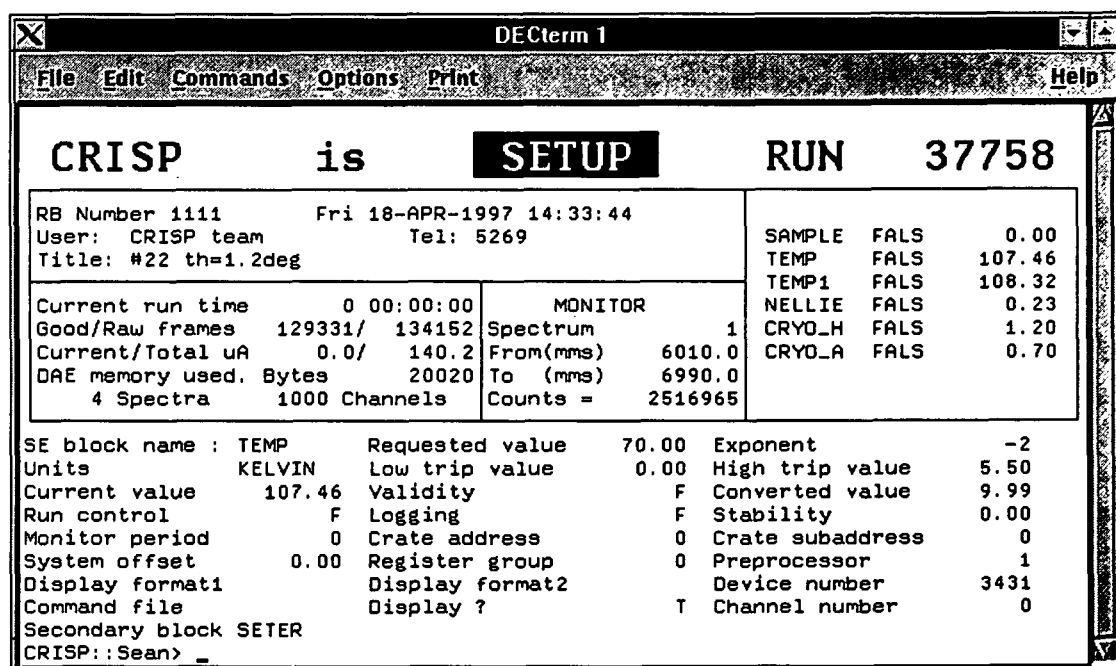


Figure 9: Dashboard showing cryostat information, in top right hand box.

To adjust the regulation temperature setpoint type `cset temp='temperature'`. To view the regulation temperature type, `cshow temp/full`. For more information on sample environment CAMAC controls see the PUNCH manual in the cabin.

3.4.3 Controlling the Centre Stick

- *Controlling the centre stick and aligning samples.*

The two axes are defined as `cryo_h` (height translation) and `cryo_a` (phi angle). The units are millimetres and degrees respectively. The alignment procedure is as described in section 3.1.2 except that the stick is controlled through the CAMAC rather than the PC the alignment does not use the SCAN command file but by running the command file: `@u:[sl.genie]scan_c`

- All the subsequent operations are identical to those in section 3.1.2. To set the position, the angle for example, simply type the CAMAC command `cset cryo_a 'angle'`. The alignment procedure needs to be performed for each of the four sample positions.

4 LOOKING AT THE DATA

The display and manipulation of the reflectivity data is all performed within the graphics package GENIE which runs from any DEC window. To run GENIE type:

\$ GENIE

Which will put you into a GENIE mode and bring up a GKS graphics window. The GENIE prompt is indicated by ». A full list of GENIE commands can be found in the PUNCH GENIE manual, copies of which are available from the ISIS computer support group. A use of some of the more common ones is found below.

Commands	Qualifiers	Description
D W{x}	/M, /L, /H	Creates new plot of specified workspace number. By default uses own limits unless these are also specified. Uses last plot option (markers, line or histogram)
P W{y}	/M, /L, /H	Plots on top of current graph specified workspace
T LOGX		Changes x scale from log to linear and vice-versa
T LOGY		Changes y scale from log to linear and vice-versa
J/P		Jump process to give use of vax without exiting GENIE.
LO		Returns to GENIE after finishing use of vax. NB this will only return to GENIE if it was exited using J/P command. If GENIE is not running this command will log-out of session.
R W{x} {filename.ext}		Reads into workspace number x the file filename.ext.
LOAD W{x} g:data_in {filename.ext}		Reads the ascii file filename.ext into workspace number x

4.1 Looking at Raw data

Soon after the run starts the raw data should be checked to ensure that the monitor is in place and the sample looks sensible.

4.1.1 Looking at Raw Single Detector Data

Within GENIE the following commands should be typed:

- » **ass dae** *Points the computer at the DAE (current data storage area).*
- » **D/H s1** *Displays the spectrum from monitor 1.*
- » **P/M s2** *Plots on top of previous graph spectrum from monitor 2.*
- » **D/H s3** *Displays on a new graph the spectrum from the detector.*

The raw data from monitors 1 and 2 have characteristic shapes as shown in Figure 10. The data from the detector varies depending on the sample but should be more intense on just background noise even after a few microamps of measurement. Your local contact will advise you.

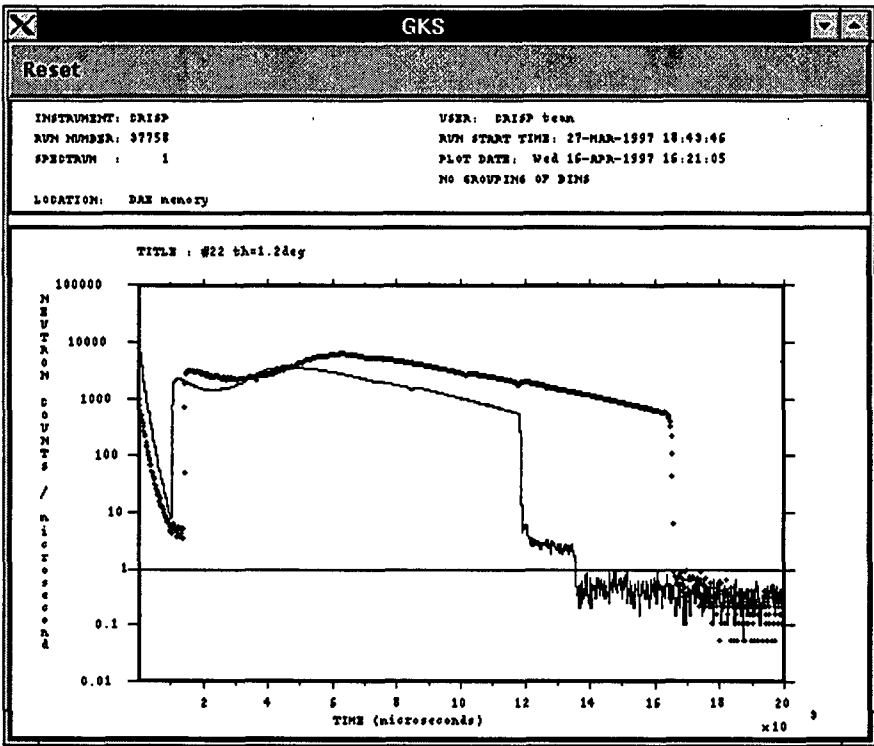


Figure 10: Typical plots of S1 (line) and S2(points) spectra raw data.

When in polarised mode there are either two or four periods, one for each spin state depending whether PA is used. The data from all the periods are all held in spectrum

within one specific run number. The spectra number for the PNR modes are shown below:

Monitor	Normal PNR	PA-PNR
Monitor 1	S1 & S6	S1, S6, S11, S16
Monitor 2	S2 & S7	S2, S7, S12, S17
Detector	S3 & S8	S3, S8, S13, S18

4.1.2 Looking at Raw Multidetector Data

The monitors 1 and 2 can be checked in the same way as for the single detector. However the multidetector creates too much data to be able to look at in the same way and it is necessary to create a '.SAV' file using UPDATE and STORE commands as indicated above. The raw data consisting of intensity versus position on the detector can be obtained by running:

» M

This asks for the run number. For the raw data from the current run, the run number with a .SAV extension should be input. Most of the other inputs can be input via a file called MULTIDET_INPUT.DAT, a copy of which must be in the directory from which GENIE was started. A sample session is shown below

```
>> m
>> @C0:[CRISP.MENU_STUFF]MULTIDET
>>   Enter OUTPUT workspace ==> :  w10
>>   ENTER RUN NUMBER ==> :   37700
>> ASS 37700
>> W1=S100
WN Parsing Buffer
WN has parsed buffer successfully
Load   Spectrum 100 into Workfile   1
Spectrum 100 is from the default file
>> TRANSFORM w1 c0:[crisp.menu_stuff]multidet w10
***** THIS VERSION FOR RUN NUMBERS >14000 *****

Input from file multidet_input.dat (1) or keyboard (2)
1
    Background file subtraction (0/1)?

    Reading file INST_DATA:CSP37700.RAW
FILE OPENED
.
.
.
Data written to workspace

    Choose another output option? (1/0)
>> INPUT workspace used = W1
>> OUTPUT workspace containing multidetector plot = w10
>>
```

To find the peak position and hence the exact angle of the reflected beam a peak fitting program can be used or alternatively this can be achieved by hand using a cursor:

either

» **D/M W{x}** *The workspace containing the data must be displayed first*
 » **pk {min} {max}** *Gaussian peak fit from minimum to maximum positions*

or

» **C/H** *Cross - hair cursor*

4.2 Reducing Raw Data to Reflectivity

Reflectivity is simply the ratio of reflected intensity divided by incident intensity as a function of wavelength or more often Q . The reduction programs used on CRISP take the TOF data from the incident monitor and the detector data and convert these to reflectivity. The efficiency of the monitor and detector are also taken into account, the ratio performed and the conversion from time to wavelength and hence Q carried out.

Several reduction programs exist to do the reduction depending on the detector used and whether using non-polarised or polarised beams:

GENIE Command	Description
QUICK	Reduces single detector data, requires input of data location (ie DAE or run number) and angle of detector.
@G:SOL	A version of QUICK for samples which uses a transmission file, ie in solid/liquid experiments, see section 4.2.1.
@G:NORM_MD2	Data reduction program for the multidetector. Requires knowledge of the peak position and exact angle.
POL	Reduces polarised neutron data giving the spin up and down in separate workspaces.
@G:POL_CSP_PA2	Version of @G:POL for full polarisation analysis, with 4 different spin states.

4.2.1 Creating a Transmission File for Solid/Liquid Measurements.

To create a transmission file for the cell, the slits should be set up as for the lowest angle measurement (approximately $S1 = S2 = 0.5$, $S3 = S4 = 2.0$) and set the detector and ϕ goniometer to 0° .

Two measurements are required:

Block transmission, *ie* Si

Air transmission, *ie* no cell

Both these data sets should be reduced using QUICK using a non-zero dummy angle. The R vs λ from each should be kept in different workspaces. The cell transmission file is obtained from the ratio of the block to air transmissions, *ie*:

$$\gg W(x) = W(Si)/W(air)$$

The final ratio should be written to a binary file as specified in section 4.6

4.3 Rebinning Data

The reduced data can be tidied up and truncated using the REBIN command. This has two modes of use:

either

`\gg REBIN W{x} {qmin} [y] {qmax}`

or

`\gg REBIN W{x} {qmin}:{qmax}`

In both cases {x} is the workspace number where the data is held ({x} = 1-50). {qmin} and {qmax} are the minimum and maximum Q values for truncating the data and y the percentage of Q data values for combining. Typical examples are:

`\gg REBIN W10 0.008 [0.02] 0.06`

or

`\gg REBIN W10 0.008:0.06`

In both cases the data from workspace 10 is taken from $Q=0.008 - 0.06$ and rebinned. In the first case with a 2% rebin and in the second case without altering the data set within these limits. When 2 or more data sets have been collected the Q range must be chosen so that there is overlap between them.

4.4 Combining Data Sets

Once the rebinning process has been completed the data sets must be adjusted so that each overlaps exactly the others. This is achieved (if necessary) by a simple Y-axis translation, *ie*

```
» w10 = w10 * 1.5
```

Once all the scaling has been carried out the data sets can be combined using COMB. This program takes the data in the workspaces and adds them into a single workspace.

```
» COMB
```

The program asks for the number of data sets, and the workspace number (NB input number without using 'w'). A typical example of a COMB session is given below.

```
>> COMB
>> @G:COMBINE
>>
>> A GENIE function/Fortran program to combine data sets
>> -- Give data sets from lowest to highest Q-range.
>> -- The workspace number only is needed.
>> G J Herdman R3 RAL January 1990
>>
>> Enter no. sets of data : 3
>> Enter workspace 1 : 30
>> Enter workspace 2 : 31
>> Enter workspace 3 : 32
>>
>> Enter output workspace : 33
>>
>> show data/output=comb_temp_c.q w32
>> show data/output=comb_temp_b.q w31
>> transform w30 int:combine_data_sets w33
```

DATA READ IN	xmin	step	xmax
Q range 1	0.8400E-02	steps in dx/x	0.2000E-01
Q range 2	0.1500E-01	steps in dx/x	0.2000E-01
Q range 3	0.5000E-01	steps in dx/x	0.2000E-01

```
Step in x (1) or dx/x (2) : 2

Enter the new step length : 0.02

No. of output bins will be 126
Is this likely to overfill the workspace?
Select new step length ? y or <CR> {RTN}

Do you wish the data to be output to an ascii file ?
If so, then give the file name : {RTN}
FORTRAN STOP
>>
```

4.5 Putting Data on an Absolute Scale

The reduced reflectivity data obtained from these reduction procedures is not on an absolute reflectivity scale. There are essentially 3 methods of achieving this and depend on the sample being measured.

- *If a total reflectivity region exists*

By definition the total reflection region has unit reflectivity. The data is therefore simply scaled so this region is on $R = 1$.

- *If using a solid/liquid cell*

In obtaining a cell transmission file (see section 4.2.1), the air transmission is obtained. The high λ asymptotic value of 'R' obtained from the output of QUICK of this air transmission measurement will be the scale factor required to put the output of @g:sol (including the transmission file reduction) on an absolute scale. This can of course be checked if a total reduction region is observed.

- *If using a air/liquids*

Although the total reflection region can be observed for many liquids, in cases where one does not exist and/or where measurements are performed well away from this region a D₂O calibration is required. The scale factor obtained to a fit to a D₂O run will put all data onto an absolute scale. It is therefore essential to collect a good D₂O calibration run at the beginning of the experiment.

4.6 Writing data to file

Since the data used within GENIE is in binary format it can be saved easily as binary format using the command.

```
>> w w{x} {filename}.Q
```

To convert to ascii and save to file the following commands should be used.

```
>> fun w{x} g:data_out w{x}

Enter output file name ==> {filename}.asc

Value of xmin for output ==> {qmin}
Value of xmax for output ==> {qmax}
Data written to ASCII file
>> Error reading from transferred data file
>>
```

This program writes data to file and saves as an ascii format.

4.7 Preliminary Data Analysis

Little will be said about fitting since this is outside the scope of this manual. However, in order to get the user started below is a brief description of some of the ways to analyse the data. We have basically two separate approaches to data fitting, one operating within GENIE and the other which is VAX based using a program using maximum entropy methods written by Devinda Sivia.

Program	System	Description
MULF	GENIE	A GENIE based program that can simulate as well as fit data. Uses standard matrix methods for calculating reflectivity profiles. The fitting program allows manipulation of all parameters. Can fit or simulate λ , Q or RQ ⁴ plots.
SLAB_FIT	VAX	A Max-Ent fitting program. Requires very little prior knowledge of the sample except substrate scattering length densities and total thickness. Tries to fit first 1 layer and then incrementally more to a maximum of 20 layers.
SLAB_REFINE	VAX	A Max-Ent fitting program. Uses an input file as an initial parameter set which are manipulated. Does not vary number of layers only adjusts parameters supplied in input file.

Further details of running any of these routines can be obtained from your local contact.

5 TROUBLE SHOOTING PROBLEMS:

Before asking your local contact for help, it may be useful to check the list of problems below which are some of the most commonly occurring.

No neutrons

- *Is the shutter open?* Check shutter control box, open shutter if closed.
- *Are the choppers running?* Check chopper control box in inner part of cabin, restart chopper at cortina if necessary.
- *Is monitor 2 in place?* Check spectrum, drive monitor 2 into running position.
- *Is main neutron beam on?* Check beam on displays in ISIS hall.

Micro-control PC Problems

- *Is it low level 'grey' screen displaying?* Click on 'high level' box
- *Has the program 'crashed' into a blue program screen?* Select RUN from menu bar and START from pop-up menu.
- *Is screen in DOS mode?* Run program by typing CRISP2 in VB-CRISP sub-directory. Select RUN from menu bar and START from pop-up menu.
- *Micro-control motions have reset to all zero?* Instrument needs resetting, seek assistance.

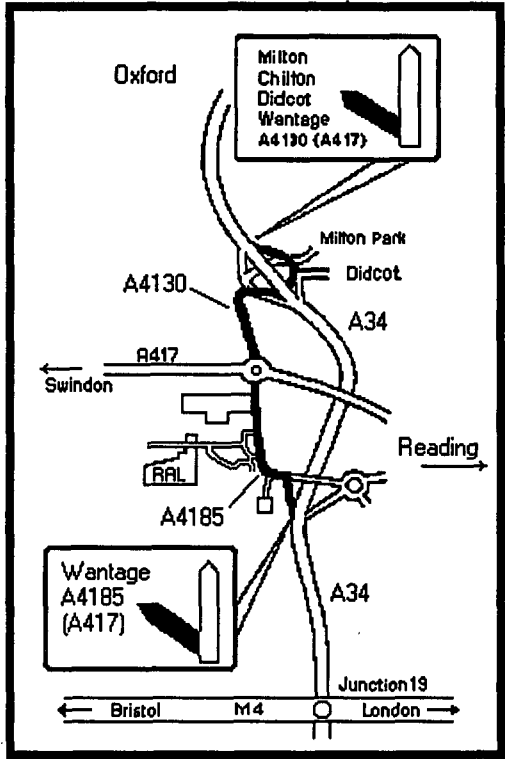
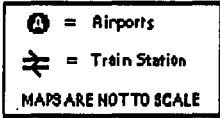
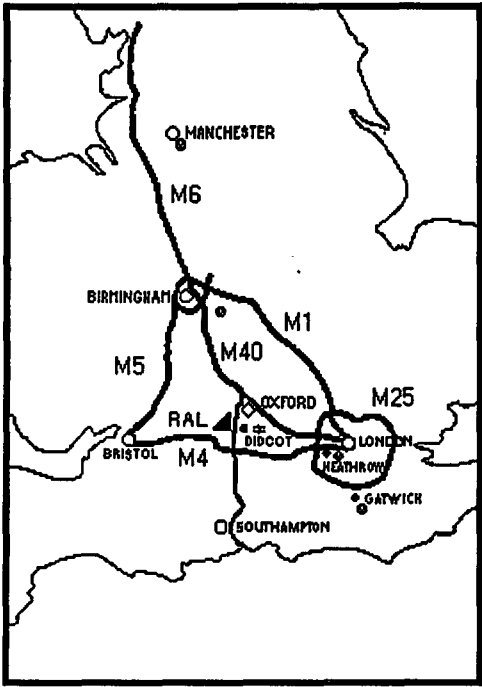
VAX Based Computer

- *Dash board has disappeared.* Try typing STAT OFF followed by STAT ON
- *Window on main computer has disappeared.* Select the *Applications* menu from the session manager and choose *Decterm* from drop down list. Input user group name to set subdirectory required.
- *Dashboard stuck in 40 periods after running SCAN.* If the SCAN program is exited at the wrong point it is possible that the correct Tables aren't loaded and the the normal single period state isn't returned. This will affect your data. Type the following to load in the correct Table

```
CRISP>copy crisp$disk0:[cspmgr.tables]sacredinst.upd
      crisp$disk0:[cspmgr.tables]inst.upd
CRISP>load crisp$disk0:[cspmgr.tables]inst.upd
```

6 GENERAL INFORMATION

■ Getting To RAL



Rutherford Appleton Lab is situated midway between Oxford and Newbury on the A4185.

By road:

Northbound: From the A34 take the A4185 (A417) exit, signposted for Rutherford Appleton Lab and Wantage. Turn left onto the A4185 and the turning for RAL is approximately half a mile from the exit.

Southbound: From the A34 take the A4130 (A417) exit signposted Milton, Chilton, Didcot and Wantage. Follow road for 1.5 miles, continue straight over roundabout onto A4185. RAL is 2 miles along on right hand side past the AEA Harwell site.

By Rail:

RAL is six miles from Didcot Parkway Station. This line is served by the Great Western intercity route from London Paddington to Bristol. Didcot also provides connections via Oxford to the Birmingham and the North, and via Reading to Stations in the South. Taxis can be found immediately outside the station.

By Air:

RAL is approximately 60 miles from Heathrow which typically takes 1 hour by car. If notified in advance users arriving at the airport can be met by a RAL representative for transporting to the lab.. This must be arranged well in advance with the University Liaison Secretariat (ULS). Alternatively, there is a half hourly Railair coach link to Reading train station where trains to Didcot depart regularly.

■ Catering Services at RAL (taken from RAL web page)

The catering services at Rutherford Appleton Laboratory are provided under contract by ARAMARK PLC. At Rutherford Appleton Laboratory ARAMARK provide the following services:

R22 Restaurant

<i>Breakfast</i>	Monday to Friday	07.30 - 08.30
	Saturday and Sunday	08.00 - 09.00
<i>Lunch</i>	Monday to Friday	11.45 - 13.45
	Saturday and Sunday	12.00 - 13.00
<i>Evening Meals</i>	Monday to Friday	17.15 - 19.15
	Saturday and Sunday	18.00 - 19.00

Customers arriving between 19.15 and 19.30 on weekdays will be offered a meal, but the choice may be limited. The restaurant and servery area will be locked at 20.00. Customers are requested to cooperate in enabling the catering staff to clear up by this time.

The lunchtime service consists of:

- Salad Bar - *self service*
- Soup & roll - *self service*
- 2 main hot counters each providing: 4 main dishes (including one vegetarian dish), a choice of hot vegetables and potatoes, and a selection of hot sweets.
- Cold sweets, cheese; biscuits, cold drinks and fresh fruit.
- Pasta Bar - *Wednesdays only*
- Baked Potato Bar - *Tuesdays and Thursdays*
- Grill Bar - *call order service providing omelettes and grills*

Healthy eating is actively promoted - look for the *Treat Yourself Right* labels. Special diets will be catered for provided adequate notice is given to ARAMARK on ext 6291 or 6229.

R22 Coffee Lounge *Mon to Fri 11.30 - 13.45*

Sandwiches, filled rolls, cakes, confectionery, hot and cold beverages.
Sit-in or take-away.

R22 Shop *Mon to Fri 08.00 - 09.30 and 11.30 - 13.45*

Newspapers, magazines, confectionery, toys, gifts, chemist, greeting cards,
postcards, postage stamps, ice-creams, cold drinks.
Sandwiches - 08.00 - 09.30 only.

R1 Coffee Lounge *Mon to Fri 09.00 - 15.45*

Hot and cold beverages, confectionery, fresh fruit - available from 09.00. Sandwiches,
filled rolls, cakes - available after 09.30 only.

Vending Machines

There are vending machines around site mostly offering beverages only. However, in the ISIS Experimental Hall there is a coffee room with a large selection of vending machines which provide hot and cold beverages as well as snack food and sandwiches. In addition the area also contains a microwave. This area is open to any ISIS user to relax away from the instrument.

■ Alternative Watering Holes

Many of the surrounding villages have pubs which serve both lunch and evening meals. A list is included to get the user started together with some of the nearby restaurants that have been frequented by previous users. Transport is almost always required (only a few hardy walkers would try to reach any but the pub in Chilton).

Pubs

			
Bell Inn	Wantage	01235	763718
Blewbury Inn	Blewbury	01235	850496
Crown & Horns	East Isley	01635	281205
Cherry Tree	Steventon	01235	831222
Fleur-de-Lys	East Hagbourne	01235	813247
George & Dragon	Upton	01235	850723
Hare Inn	West Hendred	01235	833249
Harrow	West Isley	01635	281260
Horse & Harrow	East Hagbourne	01235	850223
Lamb Inn	Wantage	01235	766768
Pack Horse Inn	Steventon	01235	831231
Rose & Crown	Chilton	01235	834249
Royal Oak Inn	Wantage	01235	763129

Swan	Wantage	01235	769238
Wheatsheaf	East Hendred	01235	833229

Restaurants (R) /Take Aways (T)

Chokkar Tandoori (T/R)	Didcot	01235	812796
Il Camino (R)	Abingdon	01235	532211
Istanbul Takeaway (T)	Didcot	01235	814210
Jade Palace (T)	Wantage	01235	762832
McDonald's (T)	Milton	01235	832212
Pack Horse Inn	Steventon	01235	831231
Pizza To Go (T)	Didcot	01235	819000
Prince of India (T)	Didcot	01235	819555
Smarts (F & C) (T)	Didcot	01235	812898



■ Applying for Beam Time

Applications for beamtime on the 15 neutron and 3 muon instruments at ISIS are encouraged from scientists and engineers from the United Kingdom and from Partner Countries. Beamtime will continue to be available for excellent proposals independent of geographical origin. Special access for industry can be also arranged.

Applications should be made by completing the form ISIS1. There are two proposal rounds each year with closing dates of 16 April and 16 October. Applications for beamtime will be recommended for scheduling by ISIS scheduling panels which meet in the first week of June and the first week of December.

Applications for Director's Discretionary time may be submitted to Dr Andrew Taylor at any time. Please note that there are new arrangements for supporting EPSRC Programmes at ISIS.

■ Useful Contact Numbers

		
David Bucknall (<i>CRISP Instrument Responsible</i>)	6437	273
Sean Langridge	5269	280
John Webster	6381	201
Jeff Penfold (<i>Head of LSS Group</i>)	5681	187

Andrew Taylor (*Head of ISIS*)

Computer Support	3029
Emergency (<i>Fire and Ambulance</i>)	2222
Health Physics (<i>Sample monitoring</i>)	6696

Main Control Room	6789
Occupational Health	6666
University Liaison Secretariat (<i>Mary and Rachel</i>)	5592
Peter Phillips (<i>Technical support</i>)	3260
Jimmy Chauhan (<i>Cryostat</i>)	3252
Zoe Bowden	3254
Dave Wootton (<i>Cortinas</i>)	6276
Trevor Cooper (<i>Choppers</i>)	3344
John Bones (<i>Electrical</i>)	3265
Hari Shah (<i>Electrical</i>)	3342

APPENDIX

■ Further Reading (A brief bibliography of some useful material)

1. DG Bucknall and JS Higgins *to be published in Recent Research Development in Polymer Science*, Ed H Hommel, 1997
2. J Penfold and RK Thomas, *J Phys Condens Matter*, **2** (1990) 1369
3. TP Russell, *Material Science Reports*, **5** (1992) 171
4. J Penfold, JRP Webster and DG Bucknall, *Proceedings of 2nd Summer School on Neutron Scattering*, Ed A Furrer, World Scientific (1995) pg 65
5. J Penfold, *Neutron, X-ray and Light Scattering*, Eds P Lindner and Th Zemb, North Holland, (1991), pg 223
6. RW Richards and J Penfold, *Trends in Polymer Science*, **2** (1994) 5
7. RK Thomas and J Penfold, *Current Opinion in Colloid and Interface Science*, **1** (1993) 23
8. DG Bucknall, *Materials World*, **3** (1995) 593
9. G.P. Felcher, *Phys. Rev. B*, **24** (1981) 1595
10. R. Felici, J. Penfold, R.C. Ward and W.G. Williams, *RAL-87-025*, (1987).
11. J. Penfold, J. Webster and D. Bucknall, *RAL-93-018*, (1993)
12. S.J. Blundell and J.A.C. Bland, *Phys. Rev. B*, **46** (1992) 3391
13. H. Zabel, *Physica B* **198** (1994) 156
14. C.F. Majkrzak, *Physica B*, **221** (1996) 342

■ Data Reduction Sessions:

Below are example sessions of various of the data reduction programs.

QUICK

```
>> quick
>> @G:QUICK
>> QUICK.COM
>>
>> CRISP QUICK DATA REDUCTION PACKAGE
>> -----
>> Quick version of NORM
>> Rebins in 50microsec steps, 0.5 to 6.5 Angstroms
```

```

>> Normalises to PLD scintillator incident beam monitor
>> Last modified by CS, 4/12/89
>> last modified by j.p. 19/4/91   for new t0 chopper
>> last modified by j.w. 02/11/93   for new SD distance
>>
>> *****
>> *****      modified for run no >27475      *****
>>
>>
>>      ****  DATA LOCATION OPTIONS  ****
>>      1      DAE
>>      2      CRPT
>>      3      DISK FILE (eg .RAW)
>>      4      ADD Runs together
>>      *****
>>      Enter option : 3
>>      Enter run number (or file name) ==> : 35000
>>      ass 35000
>>
>>      Enter 2theta value for detector ==> : 0.5
>>
>>      Normalise to incident beam monitor, PLD scintillator type
>>      Start data reduction
>>      .
>>      .
>>      .
>>
>>      End of data reduction
>>
>> ***** DATA LOCATION *****
>>
>>      Note: Data rebinned in constant Lambda bins of           0.016333
>>      between 0.5 Angstroms and 6.5 Angstroms
>>
>>      Workspace   Spectrum           X units   Y units
>>      -----
>>      W2          Detector           Lambda    Normalised to incident beam
>>      W3          Detector           Q         Normalised to incident beam
>>
>>      End of command file
>>
>>

```

POL

```

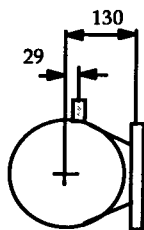
>> pol
>> @u:[sl.genie]pol_csp
>>
>>      POL_CSP.COM
>>
>>      CRISP DATA REDUCTION PACKAGE
>>      -----
>>      *****
>>      *****      modified for use for runs >27475      *****
>>      *****
>>
>>      ****  DATA LOCATION OPTIONS  ****
>>      3      DISK FILE (eg .RAW)
>>      4      ADD Runs together
>>      *****
>>      Enter option : 3      (or 1)
>>      Enter run number (or file name) ==> : 35253 (or dae)
>>      ass 35253 (dae)
>>
>>      Enter 2theta value for detector ==> : 0.6
>>

```

```

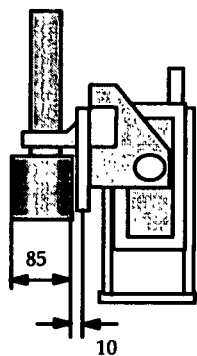
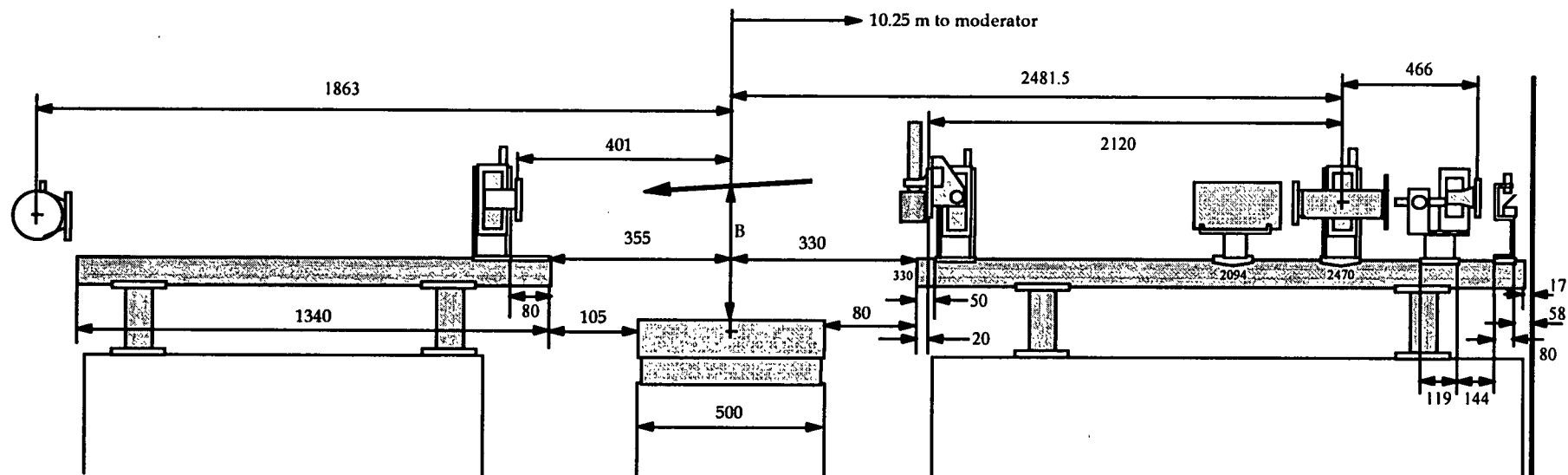
>>
>>   Enter constant bin size in time for detector data ==> :   100
>>
>>   Enter MINimum wavelength ==> :   2
>>   Enter MAXimum wavelength ==> :   6.5
>>
>> ***** MONITOR OPTIONS *****
>>     1      Helium monitor
>>     2      Magnetically shielded scintillator monitor
>> *****
>>   Enter option :   2
>>
>> ***** DATA REDUCTION OPTIONS *****
>>     1 Normalise to integrated monitor counts
>>     2 Normalise to incident beam monitor
>>     3 Normalise to smoothed (cubic spline fit) incident beam monitor
>>     4 Normalise to smoothed (polynomial fit) incident beam monitor
>> *****
>>   Enter option :   2
>>
>> ***** DATA CORRECTION OPTIONS *****
>>     1 No corrections made to data
>>     2 Corrections from latest calibration runs using run nos
>>       9162 and 9163
>>     3 Corrections from run nos 35252, 35253
>> *****
>>   Enter option :   3
>>
>> Start data reduction
>>   .
>>   .
>>   .
>>   .
>> End of data reduction
>>
>> ***** DATA LOCATION *****
>>
>> Note: Data rebinned in constant Lambda bins of           0.032667
>>        between 2 Angstroms and 6.5 Angstroms
>>
>> Corrections for polarising efficiency have been applied to all data
>>
>>   Workspace   Spectrum           X units      Y units
>>   -----
>>     W1      Flipper OFF      Lambda      Normalised to incident beam
>>     W2      Flipper ON       Lambda      Normalised to incident beam
>>     W3      FLIPPING RATIO   Lambda      W1 / W2
>>     W4      FLIPPING RATIO   Q           W1 / W2
>>     W5      Flipper OFF      Q
>>     W6      Flipper ON       Q
>>

```



CRISP Dimensions

8 May 1997

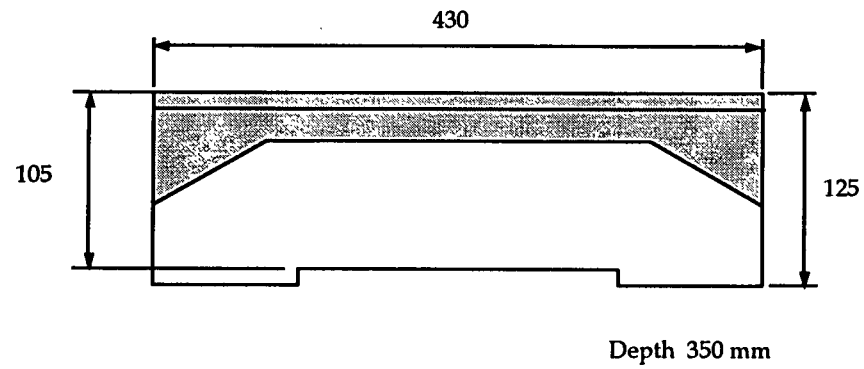


	(m)
DSM2	2.1200
DSM3	2.8660
DSM4	4.3445
DSA3	0.4010
DSA4	1.8630
DS12	2.5860

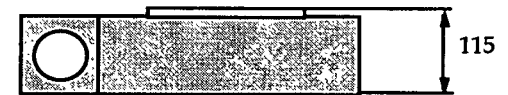
Mod - S2 9.9525 m
Mod - Det 12.1045 m

Table to Beam (B): min 236 mm
max 341 mm

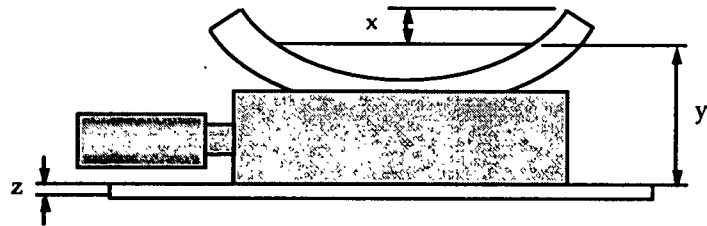
Active Vibration Table



Translator

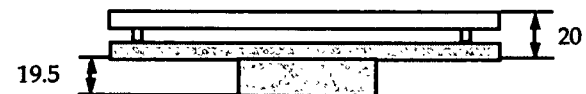


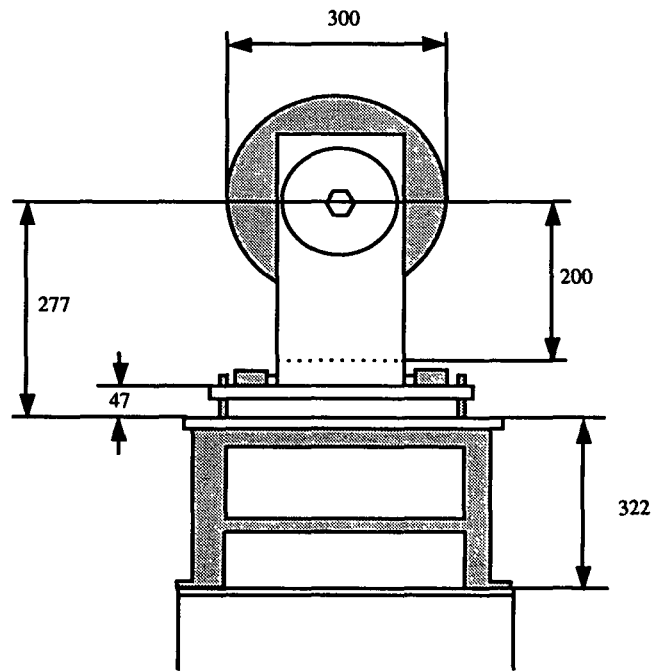
Goniometer Arcs



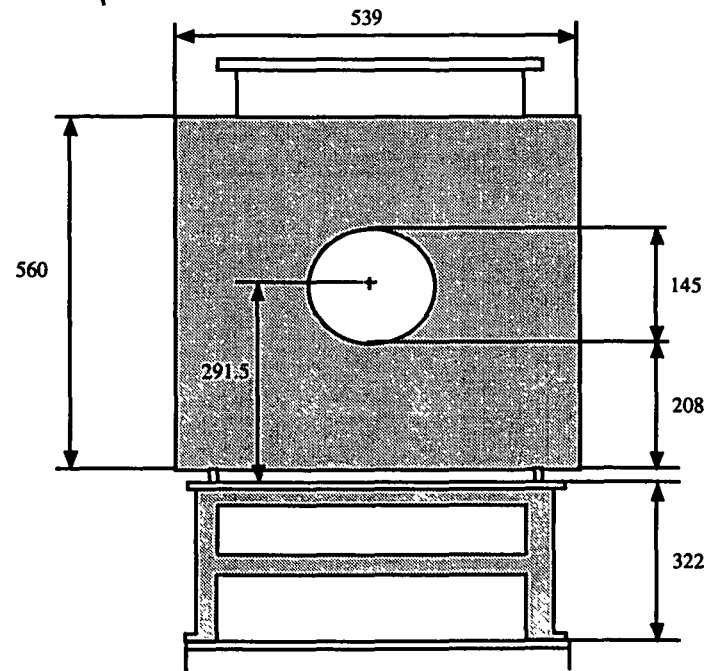
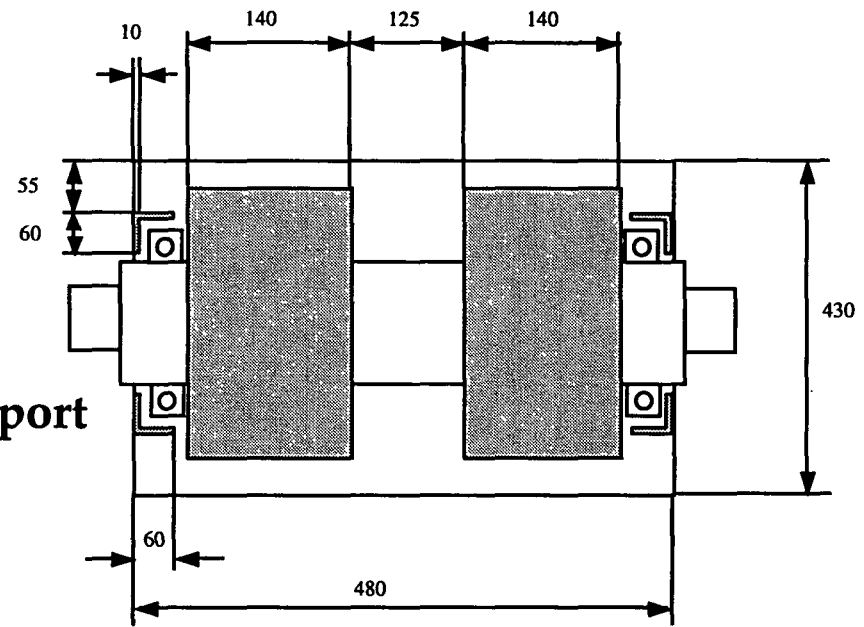
	x	y	z
BG80	43	14	---
BG120	56	---	12

Kinematic Plate





Newport

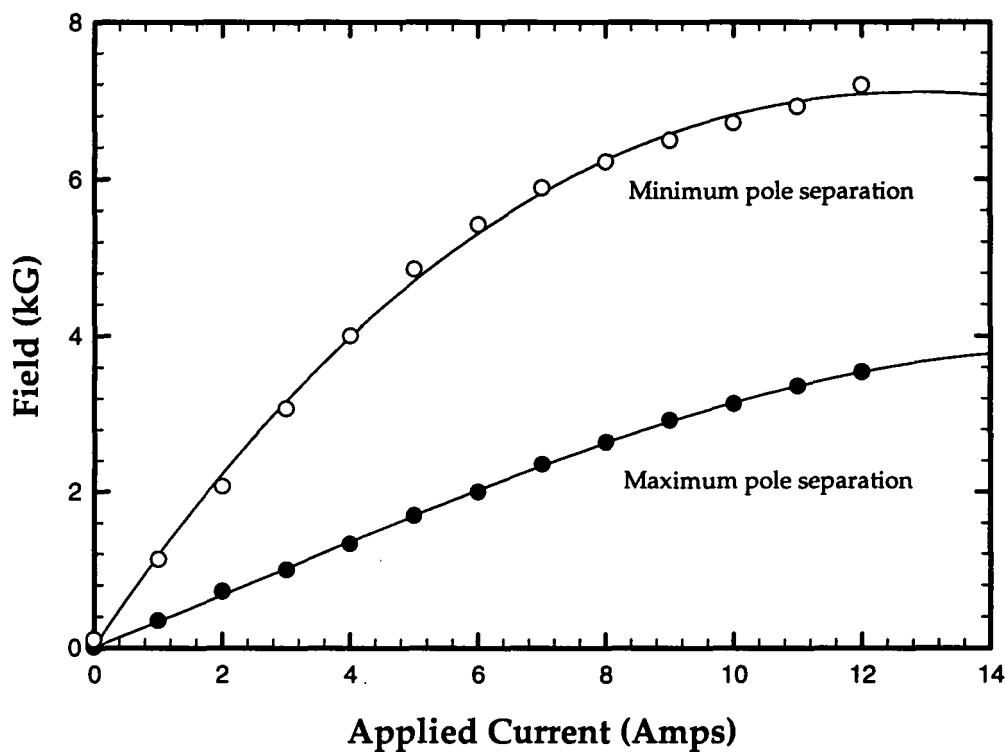


CRISP Magnets

Goudsmit

Newport Magnet

Field vs Current



Current (Amps)	Field (kG)	
	Max Separation	Min Separation
0.000	8.620e-3	0.101
1.000	0.343	1.127
2.000	0.720	2.067
3.000	0.998	3.070
4.000	1.329	4.000
5.000	1.695	4.850
6.000	1.998	5.420
7.000	2.354	5.890
8.000	2.636	6.220
9.000	2.920	6.490
10.000	3.130	6.710
11.000	3.360	6.920
12.000	3.540	7.190