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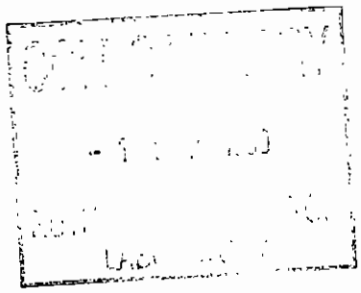
CLRC

The TOSCA I User-Guide

S F Parker D J Champion J Tomkinson and D Colognesi



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The TOSCA II User-Guide

S. F. Parker, D. J. Champion,
J. Tomkinson and D. Colognesi

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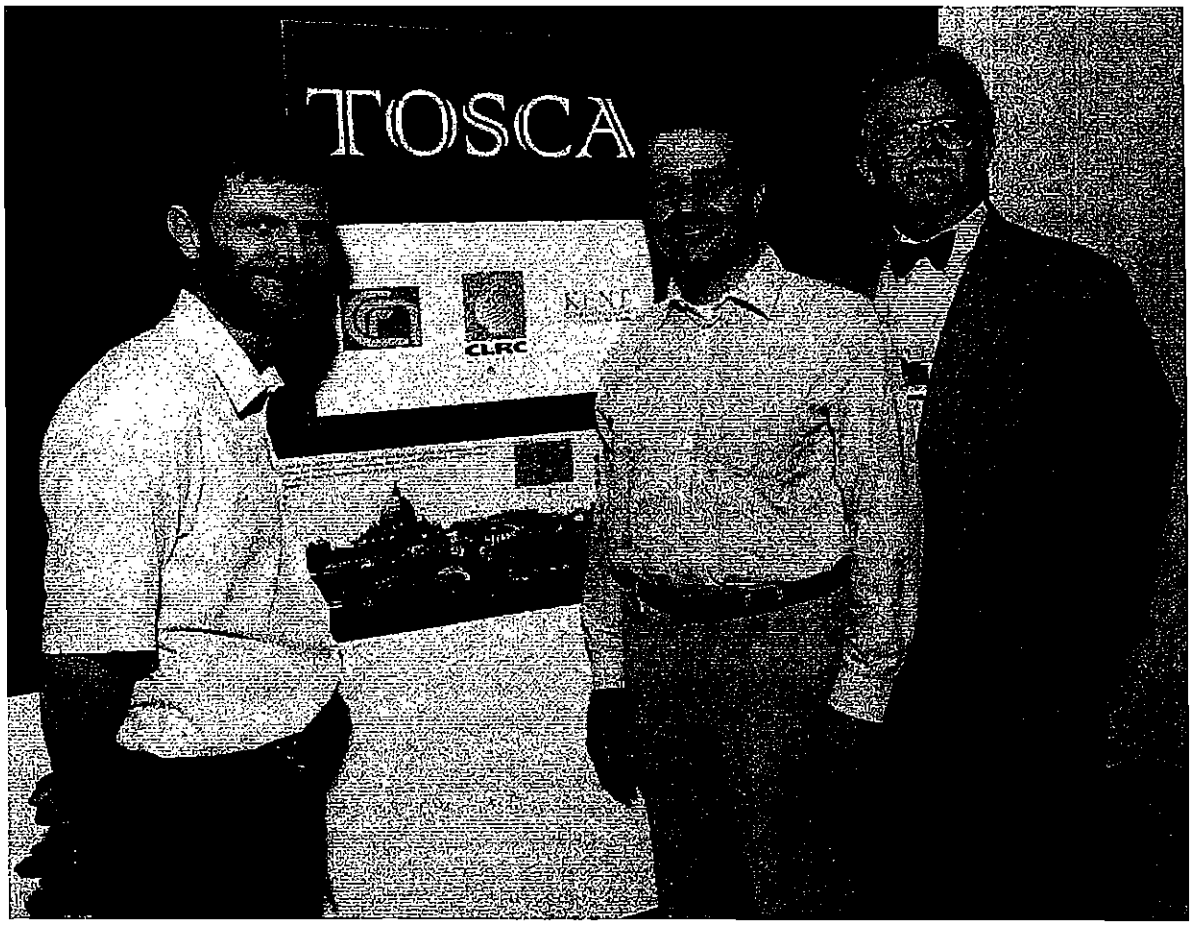
PREFACE

This document is designed as an *aide-memoire* to help you run your experiment and analyse your data. **It is not intended as a substitute for training!** For new users and those who are not regular users, it is essential that you are properly trained in the use of the instrument by your local contact or the instrument scientist.

More detailed information on some aspects is available from other reports; such as the sample environment equipment, FRILLS (a fit to a sum of Gaussian peaks) and on programs such as GENIE. Copies of these manuals can be obtained from your local contact, although copies are kept in the instrument cabin. A PUNCH manual can be found in the cabin and contains information on the Instrument Control Program (ICP) and sample environment controls via CAMAC.

This manual is specific for phase 1 of TOSCA and is also available on the web at http://www.nd.rl.ac.uk/CrystalAnalysers/tosca/toscamanual. The website version of the manual will be kept current, so users are advised to check the website if in doubt.



Team TOSCA: left to right, Stewart Parker, Daniele Colognesi (Instrument Scientists) and John Tomkinson (Group Leader, Crystal Analyser Group).

1. INTRODUCTION

TOSCA is an inelastic neutron scattering (INS) spectrometer optimised for vibrational spectroscopy. TOSCA has replaced the previous spectrometer TFXA, however, it retains the advantages of TFXA (ease of operation and reliability) but simultaneously offers improved sensitivity and resolution.

TOSCA is a collaborative project between the Consiglio Nationale Recherche (CNR) of Italy, the Department of Physics at the University of Kent at Canterbury (UK) and ISIS. (For a detailed list of the participants see the TOSCA website http://www.nd.rl.ac.uk/CrystalAnalysers/tosca). TOSCA will be installed in two phases: phase 1 was completed in May 1998 and consists of the backscattering spectrometer. at 12 m. This is similar in concept to TFXA but has 10 analyser/detector modules, see *Figure 1.1*, rather than the two on TFXA. Phase 2 will be installed in spring 2000 and will consist of the spectrometer being moved to 17 m from the source and the installation of the forward scattering detector banks and a diffraction capability. The move to 17 m, rather than the 12 m at present, will result in a large improvement in resolution.

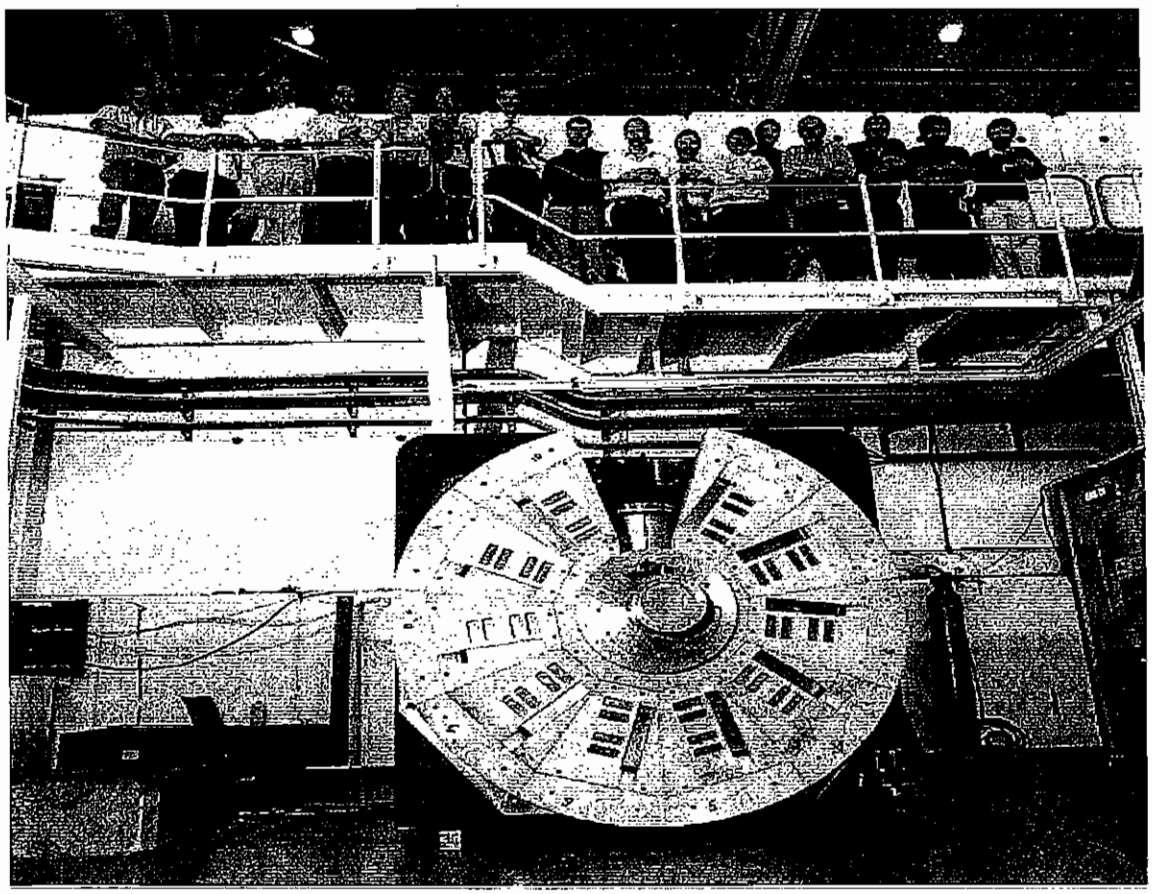


Figure 1.1. Phase 1 of TOSCA showing the detector/analyser modules.

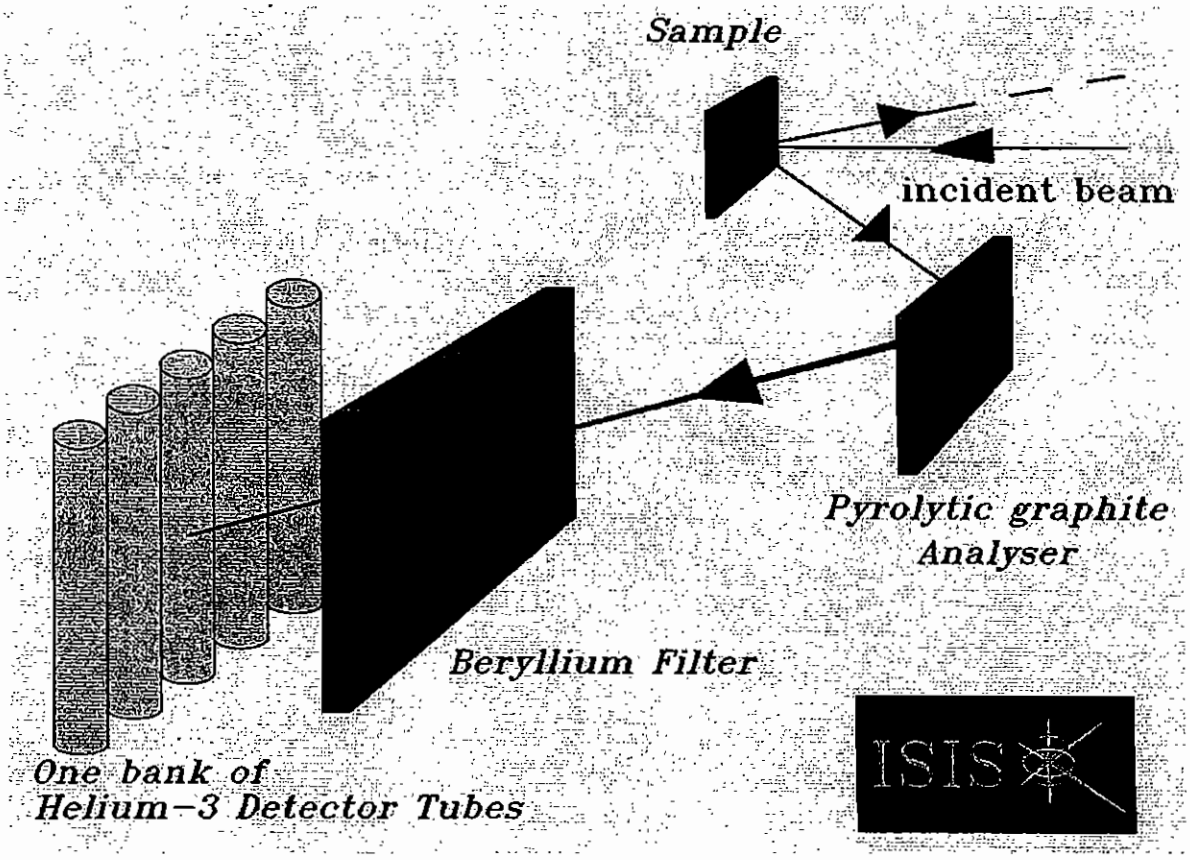


Figure 1.2. A schematic diagram of TOSCA.

TOSCA is an indirect geometry time-of-flight spectrometer at the ISIS pulsed spallation neutron source at the Rutherford Appleton Laboratory. A schematic of the spectrometer is shown in *Figure 1.2.* It is optimal in the energy range 0 - 4000 cm^{-1} (0 - 500 meV) with the best results below 2,000 cm^{-1}, (250 meV). However, data is always collected between -16 and 20,000 cm^{-1} (-2 - 2,500 meV) and may be analysed across the entire range.

The source of neutrons on TOSCA is the white beam from the water moderator. The time-of-flight technique is used for energy analysis of the scattered neutrons. A small fraction of the incident neutrons are inelastically scattered by the sample; those that are backscattered through an angle of 135° impinge on a graphite crystal. Bragg's law states:

$$n\lambda = 2d\sin\theta \qquad (1)$$

where d (Å) is the interplanar distance in the crystal, λ (Å) is the wavelength of the scattered neutron and θ is the angle of incidence on the crystal.

From equation 1, since both d and θ are constant only one wavelength (and its harmonics) will be Bragg scattered by the crystal, the remainder will pass through the graphite crystal to be absorbed by the shielding. The neutrons at multiples of the fundamental wavelength are scattered by the beryllium filter which acts as a longpass filter and the remaining neutrons are then detected by the ^{3}He filled

detector tubes. The net effect of the combination of the graphite crystal and beryllium filter is to act as a narrow bandpass filter.

The energy transferred to the sample, E_{trans}, is:

$$E_{trans} = E_i - E_f \tag{2}$$

where E_i and E_f, are the incident and final energies respectively. The kinetic energy, E, of a neutron is given by:

$$E = \frac{mv^2}{2} \tag{3}$$

where m is the mass of the neutron and v is its velocity. Rearranging (3) gives:

$$v = \sqrt{\frac{2E}{m}} \tag{4}$$

and since

$$travel\ time = distance/velocity \tag{5}$$

It follows that the time of arrival at the detector, T, is the sum of the time from the moderator to the sample, t_i, and the time around the analyser, t_f, thus:

$$\begin{aligned} T &= t_i + t_f \\ &= \frac{L}{v_i} + \frac{l}{v_f} \\ &= L \Big/ \sqrt{\frac{2E_f}{m}} + l \Big/ \sqrt{\frac{2E_i}{m}} \end{aligned} \tag{6}$$

Now since the final energy, E_f, the distance round the analyser system, l, and the length of the flight path from the moderator to the sample, L, are all known, it follows that the time of arrival at the detector uniquely defines the incident energy, E_i, and hence the energy transfer at the sample, E_{trans}. Thus it is a simple matter to convert from time-of-flight to energy. The result is a spectrometer with no moving parts than can record spectra from 0 to 8000 cm^{-1}, although the best results are usually obtained below 2000 cm^{-1}. The resolution of the spectrometer is determined by a number of factors but for practical purposes can be taken to be 2% of the energy transfer.

The intensity of the ith molecular vibrational transition is proportional to:

$$I_i \propto Q^2 U_i^2 \exp\left(-Q^2 U_{Total}^2\right)\sigma \tag{7}$$

Since neutrons have a mass approximately equal to that of the hydrogen atom, an

inelastic collision results in a significant transfer of momentum, Q ($Å^{-1}$), as well as energy, to the molecule. On TOSCA the design is such that there is only one value of Q for each energy, ($E_{Trans} \approx .\ 16Q^2$). (Other instruments at the ISIS Facility and the ILL allow both the energy and the momentum transfer to be varied, but they constitute a different story). U_i is the amplitude of vibration of the atoms undergoing the particular mode. The exponential term in equation (7) is known as the Debye-Waller factor, U_{Total} is the mean square displacement of the molecule and its magnitude is in part determined by the thermal motion of the molecule. This can be reduced by cooling the sample and so spectra are typically recorded below 50K.

σ is the inelastic neutron scattering cross-section of all the atoms involved in the mode. The scattering cross-sections are a characteristic of each element and do not depend on the chemical environment. The cross-section for hydrogen is ~80 barns while that for virtually all other elements is less than 5 barns. This means that modes that involve significant hydrogen displacement will dominate the spectrum. This dependence on the cross-section is why the INS spectrum is so different from infrared and Raman spectroscopies. There, the intensity derives from changes in the electronic properties of the molecule that occur as the vibration is executed, (the dipole moment and the polarisability for infrared and Raman spectroscopy respectively).

A consequence of the indirect geometry is that for energy transfers >100 cm^{-1} the momentum transfer vector is essentially parallel to the incident beam. The significance is that for an INS transition to be observable there must be a component of motion parallel to the momentum transfer vector. This means that with oriented samples (such as single crystals or aligned polymers) measurements directly analogous to optical polarisation experiments carried out .

In addition to the inelastic detectors there are also two ^3He filled detector tubes either side of the incident beam. These are for elastically scattered neutrons and enable modest resolution, $\Delta d/d \approx 3 \times 10^{-3}$, diffraction patterns to be recorded simultaneously with the inelastic spectrum. The purpose of the detectors is to provide a check on the crystal phase of the material and to monitor phase changes as an experimental variable is changed *e.g.* temperature and pressure. There is also a low efficiency scintillation detector (the monitor) in the main beam just before the cryostat vacuum tank. This measures the incident flux distribution as a function of time and is used to normalise the spectra.

Further reading

There is more information about TFXA and TOSCA at the Crystal Analysers website: http://www.isis.rl.ac.uk/CrystalAnalysers/. This includes a list of publications resulting from work on TFXA and TOSCA. There is also a database of INS spectra that have been obtained on the instruments. Two types of ASCII and two types of image files are available for downloading. The database is at: http://www.isis.rl.ac.uk/INSdatabase/

S. F. Parker, C. J. Carlile, T. Pike, J. Tomkinson, R. J. Newport, C. Andreani, F. P. Ricci, F. Sachetti and M. Zoppi, "TOSCA: A World Class Inelastic Neutron Spectrometer", Physica B 241-243 (1998) 154-156. This paper gives an overview of TOSCA.

S F Parker, "Vibrational Spectroscopy With Neutrons", Spectroscopy Europe 6 (1994) 14-20. This gives a brief description of TFXA (very similar to the one given here!) and highlights some of the areas of current research on the instrument.

J Tomkinson, "The Vibrations of Hydrogen Bonds", Spectrochimica Acta, 48A (1992) 329-348. Illustrates the application of INS to hydrogen bonding studies.

G J Kearley, "A Review of the Analysis of Molecular Vibrations Using INS", Nuclear Instruments and Methods in Physics Research, 354 (1995) 53-58. An excellent overview of how to fully analyse INS data using normal coordinate analysis.

J Tomkinson, "Neutron Molecular Spectroscopy", in *Recent Experimental and Computational Advances in Molecular Spectroscopy,* (R Fausto ed.) Kluwer, 1993 pp229-249. Briefly describes the theory of INS (and references to in-depth treatments) and some applications.

1.1 Sample Environment on TOSCA

The beam size at the sample position is 50 mm high by 20 mm wide. It is clearly advantageous to fill as much of the beam as possible. For the best resolution the sample should be 1 mm thick, however, samples up to 4 mm thick are usable.

Solid samples are usually just wrapped in aluminium foil and attached to a centrestick (see section 2.4 Preparing samples). Liquid samples are run in thin walled aluminium cans. Air or moisture sensitive samples (solid or liquid) should be loaded into the cans in a glovebox.

As explained in the previous section, to maximise the INS intensity it is necessary to reduce the Debye-Waller factor as much as possible, thus virtually all samples on TOSCA are cooled. Cooling below 50K makes little difference to the spectrum, thus a Closed Cycle Refrigerator (CCR) which attains temperatures below 20K region is adequate for most samples, see *Figure 1.3*. This has the virtues of being reliable, cheap to run and simple to operate. The CCR is isolated from where the sample sits and uses helium exchange gas to cool the sample. This has the advantage that the sample can be changed without warming the CCR, thus samples can be changed in a matter of minutes without difficulty. Further details are given in section 3.2.1.

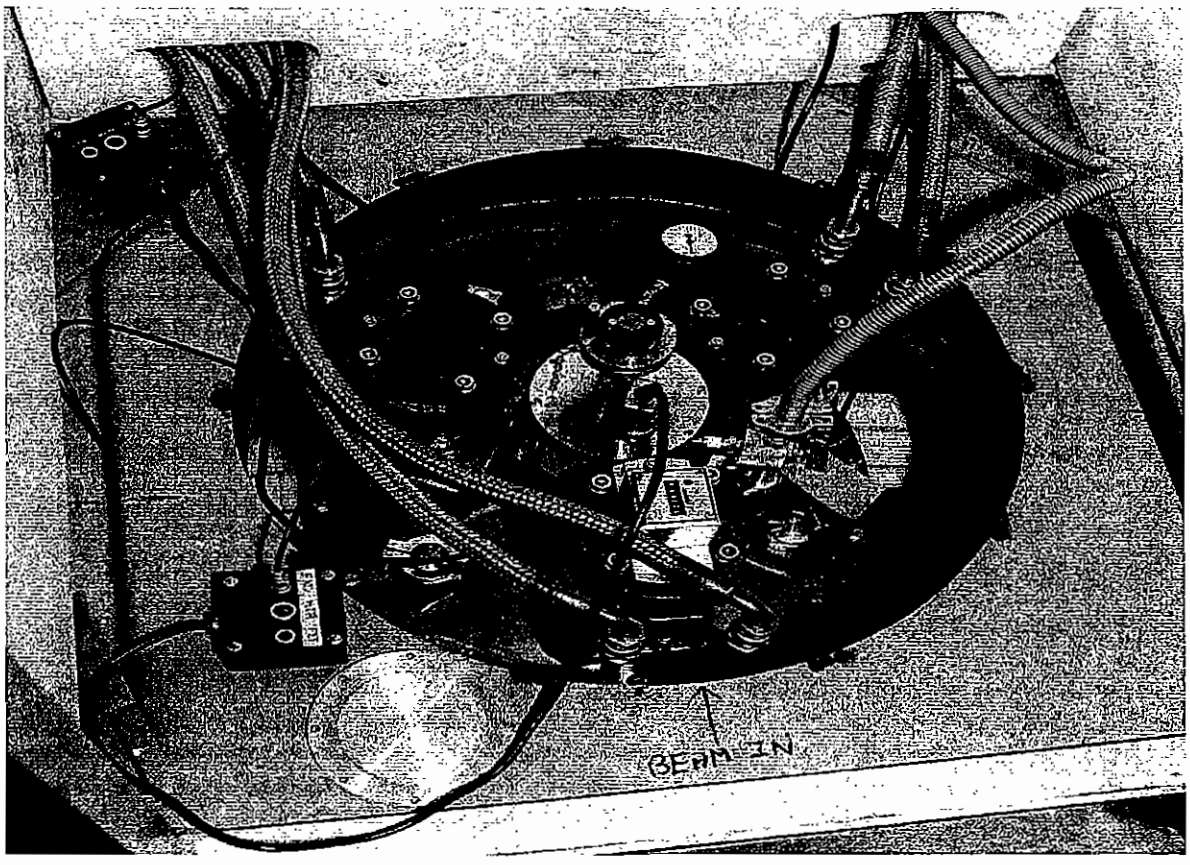


Figure 1.3: Top loading CCR on TOSCA.

The TOSCA CCR has a an internal diameter of 100 mm so will take standard ISIS centresticks. In addition, there are a number of dedicated centresticks for special applications. There are two centresticks that enable 4 samples to be loaded simultaneously, see *Figure 1.4* and section 2.3. One of these may be operated under computer control.

If temperatures below the base temperature of the CCR (~ 20K) are required then normal ISIS practice would be to replace the CCR with a liquid helium cryostat ("orange cryostat"). Because of space constraints this is not possible on TOSCA. Instead, there is a centrestick that incorporates a liquid helium bin in its shaft. The design is such that it holds sufficient liquid helium to enable a spectrum to be recorded, see *Figure 1.4*. It may also be pumped on to give a base temperature of ~ 1.5K. This is currently (Spring '99) being commissioned. It is available for use but must be requested well in advance of the experiment (a minimum of two weeks and ideally on the proposal form).

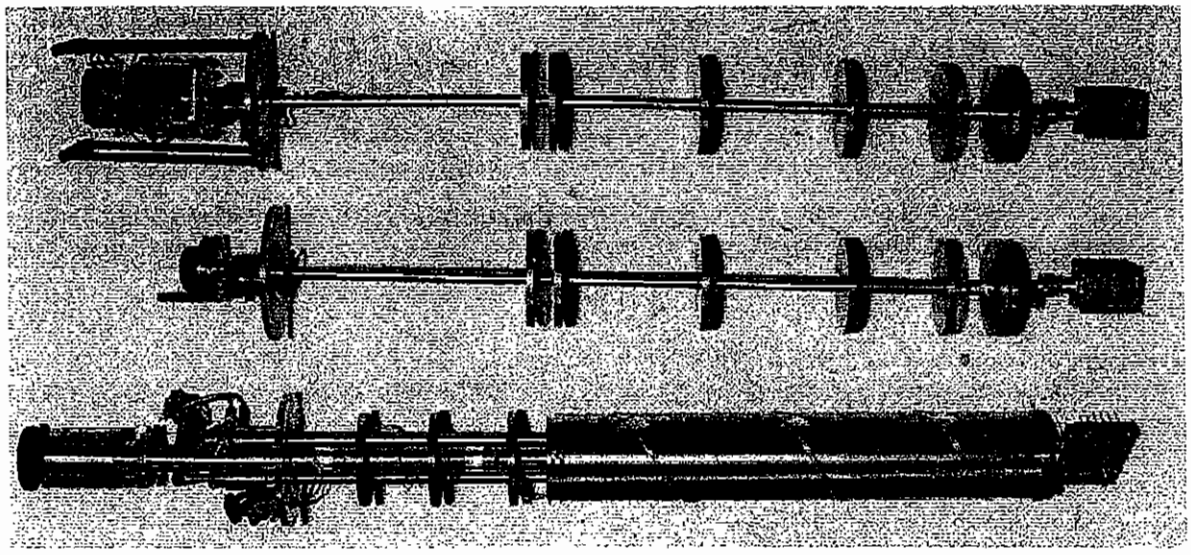


Figure 1.4: The motorised (top), manual (middle) 4-position centresticks and the liquid helium centrestick (bottom) for use on TOSCA.

For pressure experiments there are two options. For pressures up to 4 kbar, the helium intensifier should be used. This allows relatively large samples (the can is 7 mm diameter x 40 mm long) to be used and the pressure can be adjusted with the centrestick in the beam. For higher pressures, the McWhan Clamped Cell is used. The McWhan cell, see *Figure 1.5*, uses pre-stress alumina inserts to achieve pressures of up to 25 kbar. The sample sizes are of the order of 4 mm in diameter and 10 mm long. It is not possible to pressurise in-situ, and it takes several hours to cool the whole cell once it is on the instrument. **If experiments at pressure are intended then the equipment must be requested on the proposal form. It is not available on demand.**

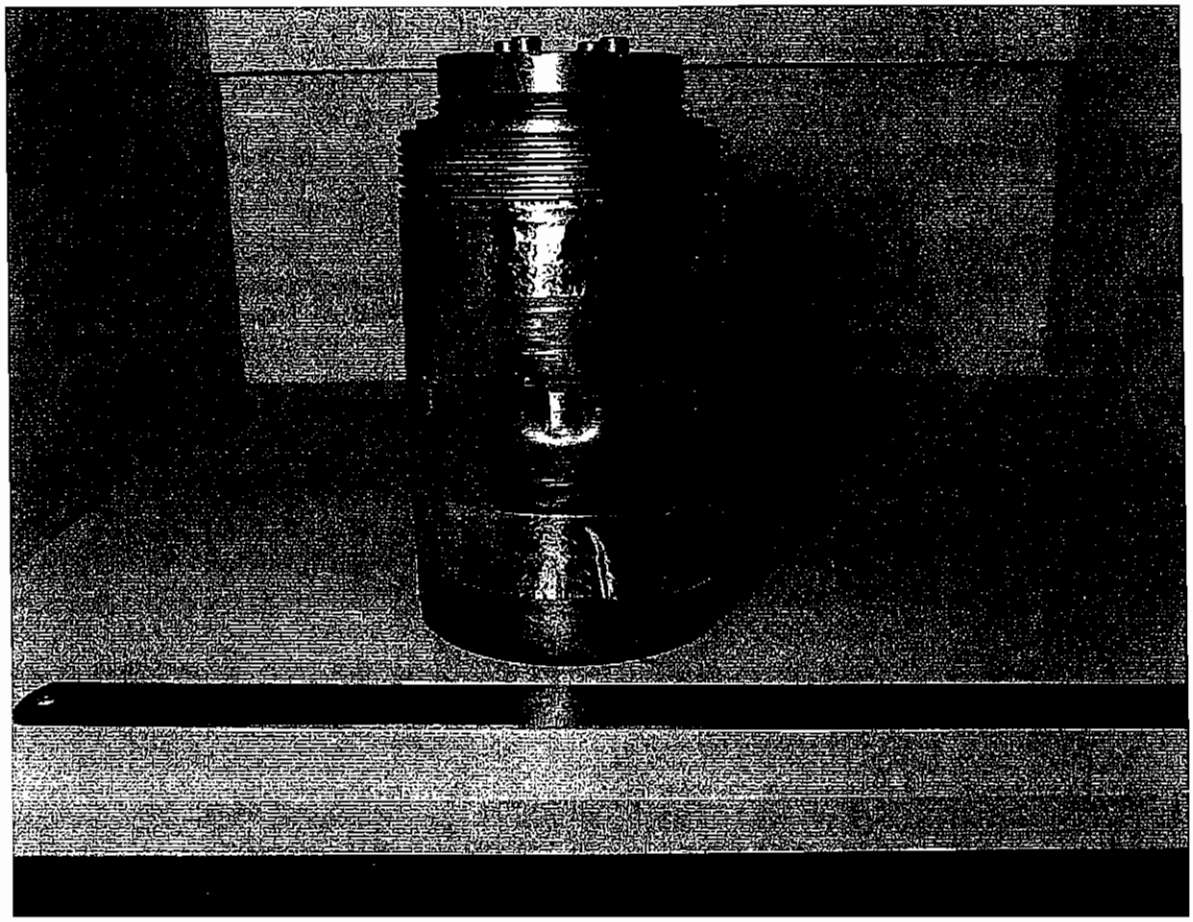


Figure 1.5: McWhan Cell *95RC3075*

2. RECORDING A SPECTRUM

This section describes how to prepare a sample, load it into TOSCA and what to do if a centrestick sticks in the instrument.

2.1 Safety

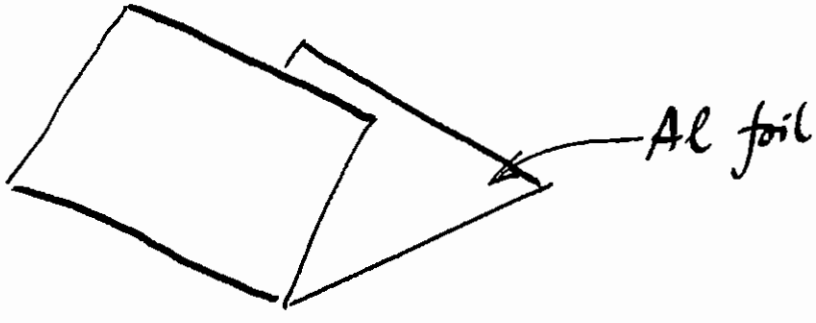
There are a number of safety issues associated with work at ISIS. The most obvious is the radiation hazard from the neutron beam and from irradiated samples and sample environment equipment. This is minimised by the use of interlocks, monitoring the radiation levels and appropriate handling and storage of irradiated materials. ***If in doubt, ask*** (your local contact, Health Physics or the Main Control Room). **Before you start an experiment you must watch the ISIS safety video** (in either the DAC or the coffee room in R3) and sign the yellow card. There is also the risk of exposure to chemicals, in this case the handling instructions on the back of the sample sheet state the required procedures to follow. Note that cadmium metal is toxic (it also activates in the beam) so should be handled with care. On removal from a cryostat, samples and centresticks are usually very cold, so should not be handled without gloves. Some of the sample environment equipment is heavy or bulky, so should be carried with due respect.

2.2 Preparing samples

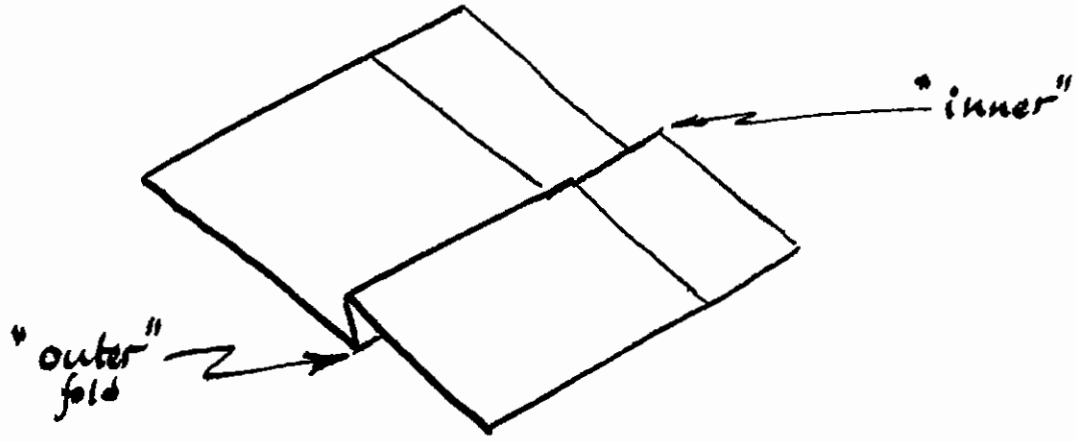
The laboratory's official handling instructions will be found on the back of the sample requirement form. You are required to observe them. For solids the easiest way to present the sample is to load it into an aluminium foil sachet. These are constructed as described in section 2.2.1. For liquids, a thin walled aluminium can is used. The same containers can be used for air or moisture sensitive samples, except that the can is loaded in a glovebox.

2.2.1 Preparing an aluminium sachet

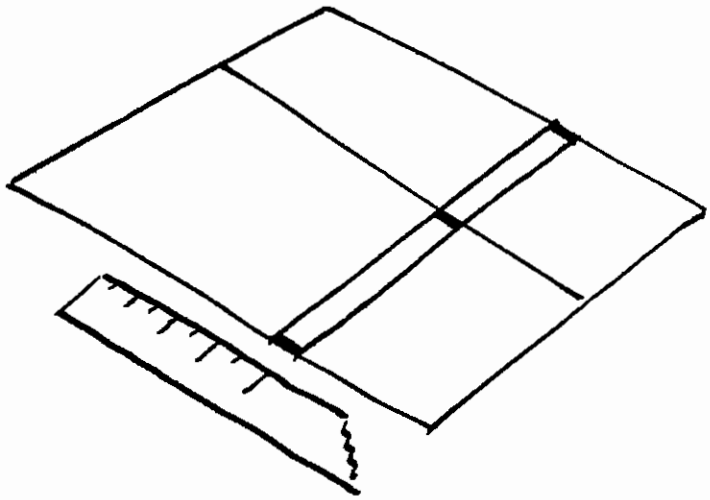
1. Tear off a piece of foil 20 cm long and fold it over



2. 1st 'Z' fold on right-hand side

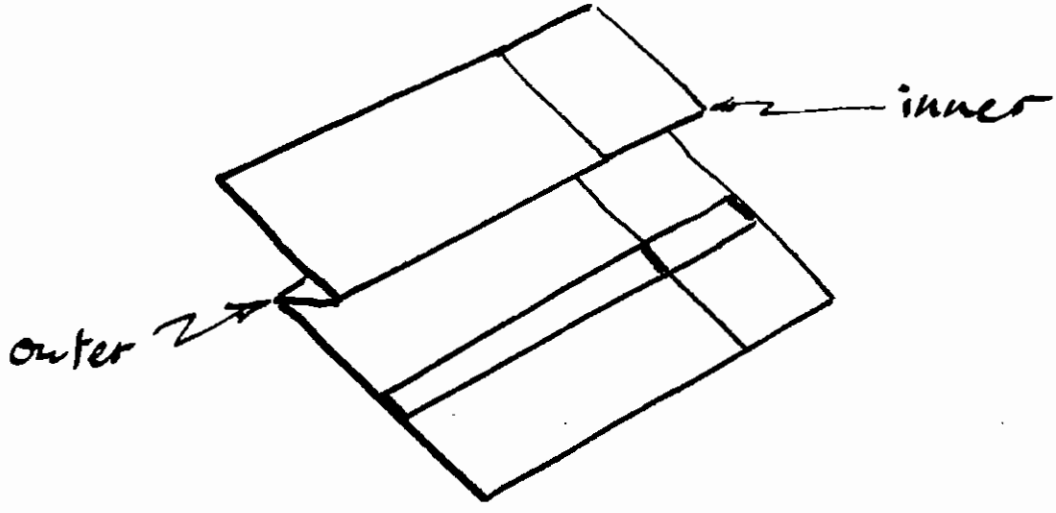


3. Press 'Z' fold flat, using back of fingernail, or plastic ruler.



4. From "outer" fold mark off sachet width (this is normally 20 mm; however, for bulky samples this must be ~30 mm).

5. 2nd 'Z' fold, on left-hand side

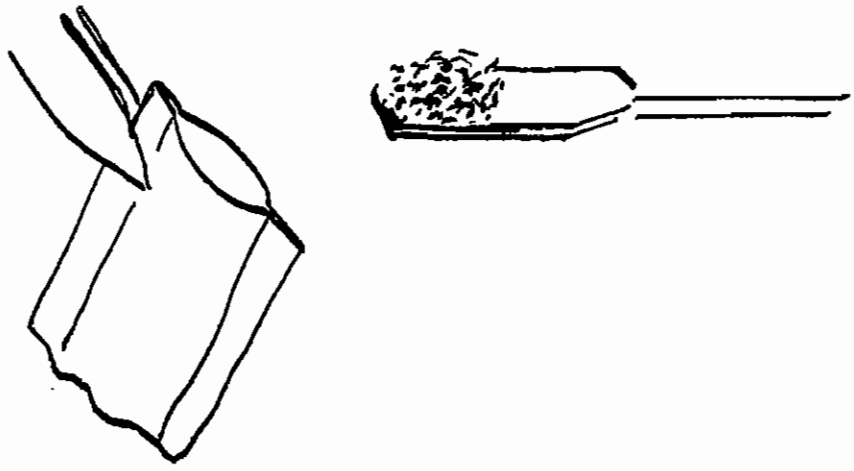


6. Press Z fold flat and cut away excess foil from the sides.

7. Hold the 'Z' folds, one in each hand, tightly between finger and thumb close to the mouth of the sachet. Blow briefly and not too strongly into the sachet mouth.

   If done correctly the sachet opens like a paper bag ready for filling. If overdone the Z folds will become undone. (Alternatively, a pencil or other blunt instrument also works!).

8. Fill the sachet



9. Tamp the sample gently to the bare of the sachet. Close off the sachet immediately above the sample using finger and thumb.

10. At a height of 50mm from the base of the sachet, fold a few times to seal.

11. The sample should be evenly distributed throughout the sachet using a cylindrical bottle like a "rolling pin". The finished article should resemble the sachet in *Figure 2.1.*

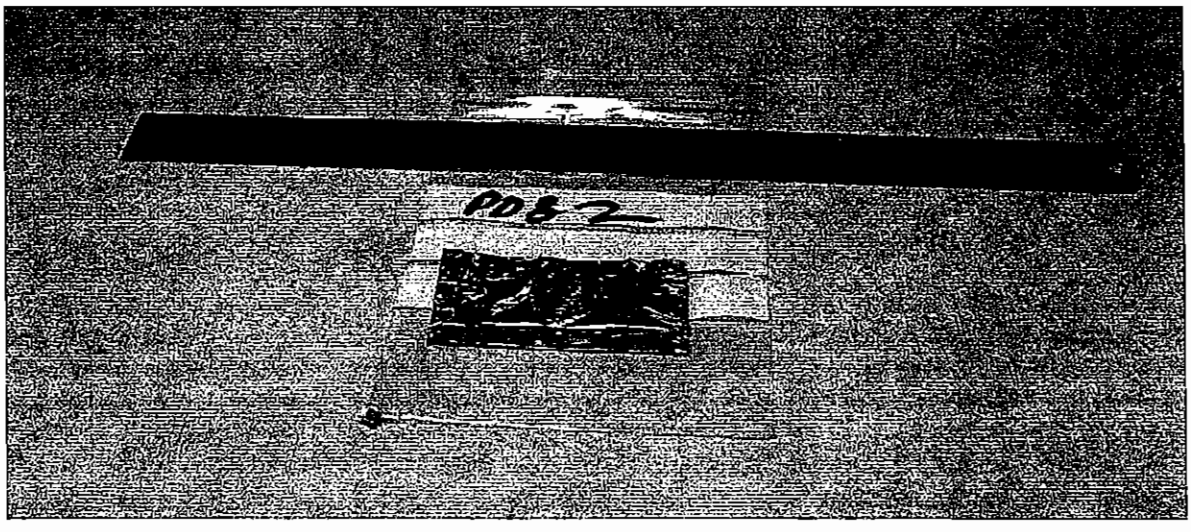


Figure 2.1: Picture of sachet with scale

Hints

1. Using a blunt pencil the sachet can be "impressed" with a name.

2. If you have produced a sample that is too thin, DO NOT start afresh, simply make another and run both!

3. If you puncture a sachet, enclose this sachet in some Al foil which can be gripped on the centrestick as usual.

2.2.2 Loading the samples onto a centrestick.

The procedure is basically the same whether the two position centrestick is used or the four-position "lantern" centrestick *(Figure 2.2)* is used. In most circumstances, it is desirable to use the 4-position centrestick since four samples can be loaded simultaneously and the overhead in cooling the samples is greatly reduced. The beam centre is 1165 mm below the **underside** of the centrestick flange and the beam itself is 50 x 20 mm (h x w). The sample should cover as much of the beam area as possible and be preferably no more than 2mm thick. Care should be taken that only the sample and the Al sachet are in the beam; items such as sensors, heaters, tape or wire should not intrude.

With the four-position "lantern" centrestick, the samples are attached to the cadmium lantern. The rotary feedthrough on top of the flange is numbered. Note the position of each sample when it is mounted on the lantern. Either tape or wire can be used to hold the sample on the lantern. There are 4 lanterns and these should be alternated to allow the activity of the Cd lantern to decay to a safe level before the next usage. It is good practice to check the activity of the lantern before use. Occasionally, it is necessary to use a lantern that it is slightly active, in this case gloves should be worn while mounting the sample on the lantern.

There are two four-position centresticks, one of which may be operated under computer control. You should discuss with your local contact which is optimal for your experiment.

If measurements at temperatures other than the base temperature of the CCR (~20K) are intended, then the best method is to attach heaters and a sensor to the grooves at the corners of the lantern.

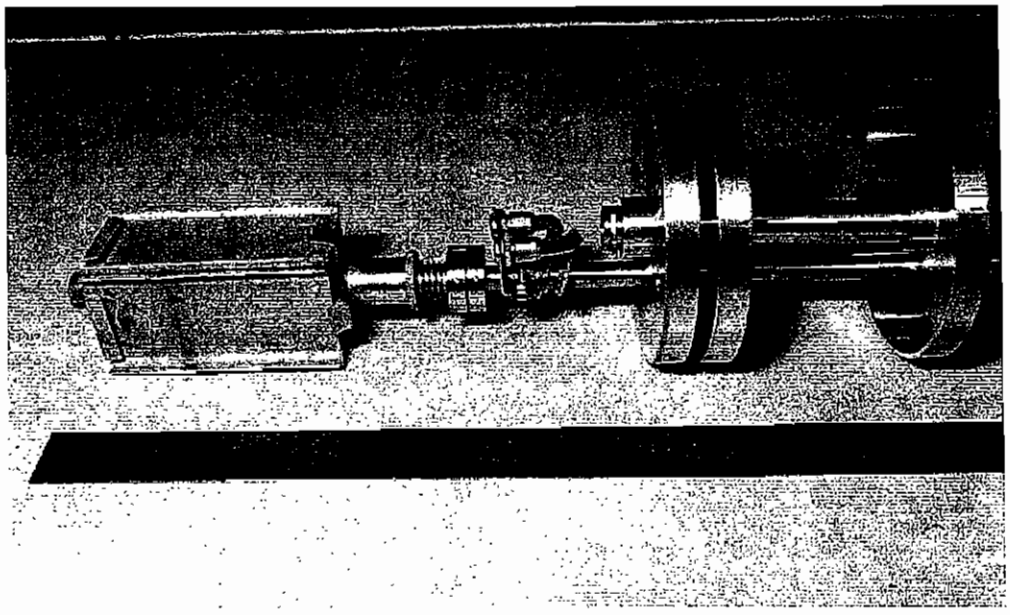


Figure 2.2: The four position Cd "lantern" mounted on the centrestick.

2.2.3 Preparing an aluminium can

For liquid or air sensitive samples a sealed thin-walled aluminium can should be used. With liquid samples the cell should be filled in a fumehood or a glovebox if sensitive to the atmosphere. For air or moisture sensitive solids, the sample should be loaded, and the can assembled in the glovebox. There are two types available. One type of cell is designed to go on the 4-position sample changer so up to 4 samples can be loaded simultaneously (these can be all cans or a mixture of sachets and cans). These have pathlengths of either 2 or 4 mm. For hydrogenous materials, the 2 mm length should be used since this is sufficient sample to give an excellent spectrum in around 6 hours. *Figure 2.3* shows one of these cells disassembled and a complete cell.

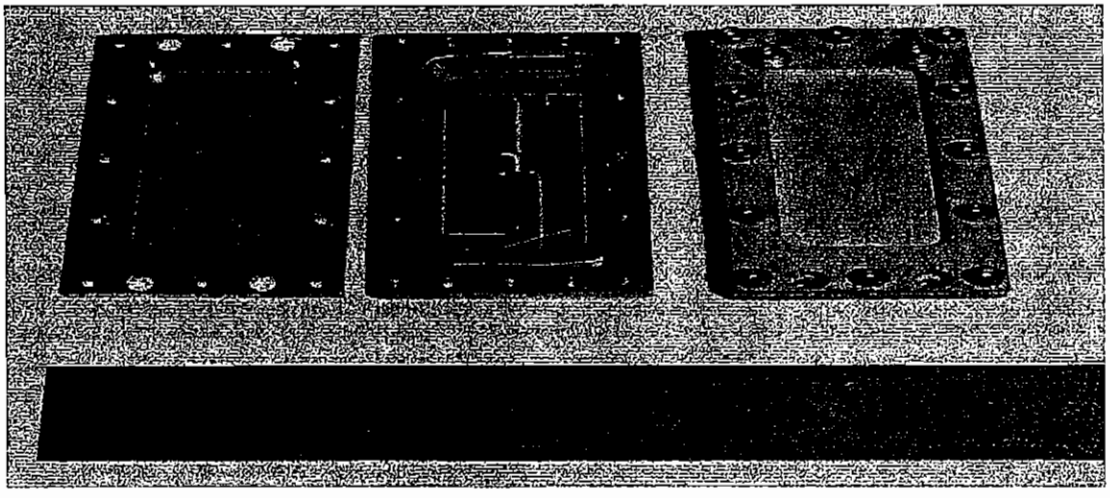


Figure 2.3: A liquid cell for the four position sample changer.

Figure 2.4 shows the second ("HET") type cell of thin walled aluminium sample can and its components. The can consists of two outer cases and a spacer. The spacer thickness can be varied between 1 and 10 mm. The can is sealed using either indium wire (narrow grooves) or with Viton O-rings (wide grooves). Since the width of the can is much greater than that of the beam, solid samples should be loaded into a sachet and this positioned in the centre of the can before assembly. To reduce scattering from the cell, it should be completely shielded with cadmium apart from the opening at the front of the cell. Owing to the large mass of the cell, once loaded and attached to the centrestick, it should be immersed in liquid nitrogen for a few minutes immediately prior to putting the centrestick in the cryostat. This reduces the cool-down time to less than an hour, from several hours.

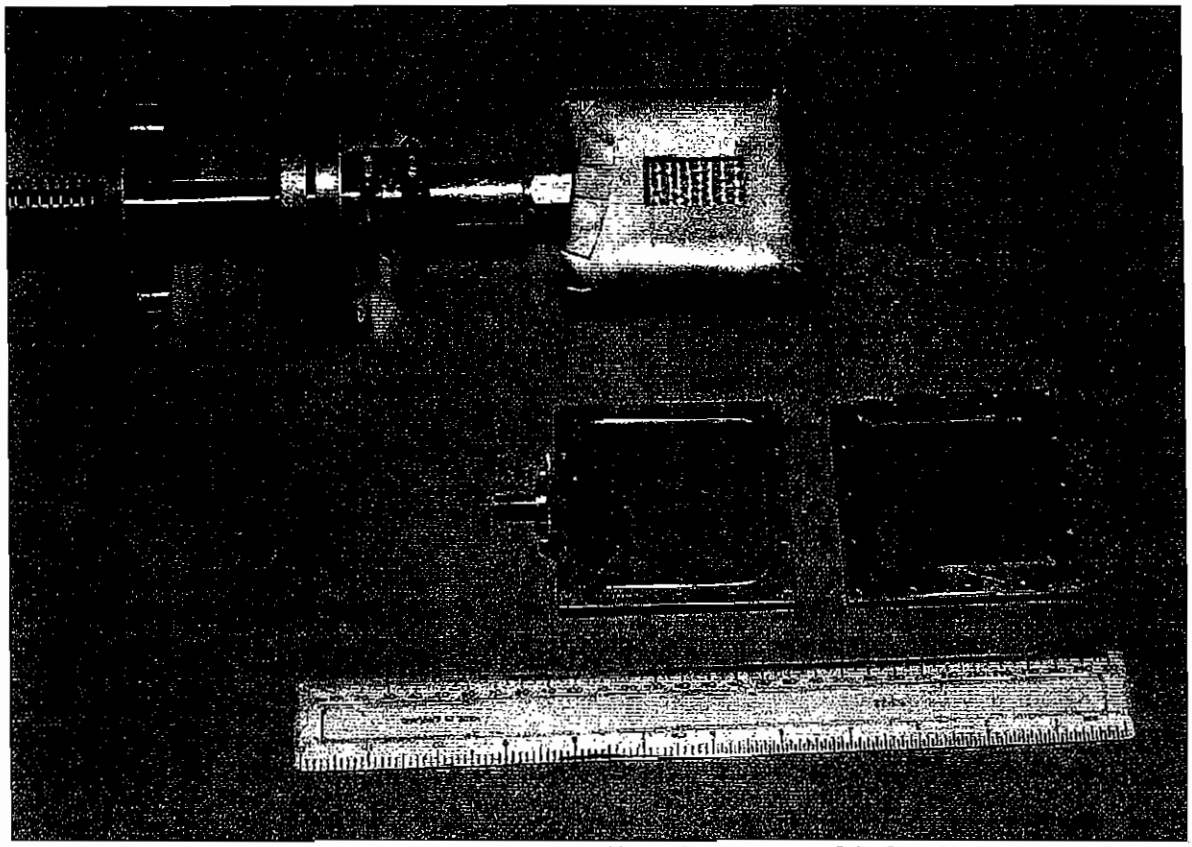


Figure 2.4: The components of a liquid cell and an assembled cell, shielded with cadmium mounted on a centrestick.

2.3 Changing Sample

Before changing a sample, familiarise yourself with the TOSCA cloche and the area around it. *Figure 2.5* shows the gate and interlocks to the TOSCA enclosure and highlights the location of the important items. The following procedure assumes that the four-position sample changer is being used. If an aluminium can or other large piece of equipment (*e.g.* a catalysis cell or a McWhan cell) is being used, then it is essential to pre-cool this in liquid nitrogen immediately before insertion into the cryostat, otherwise the cool-down time is prohibitively long.

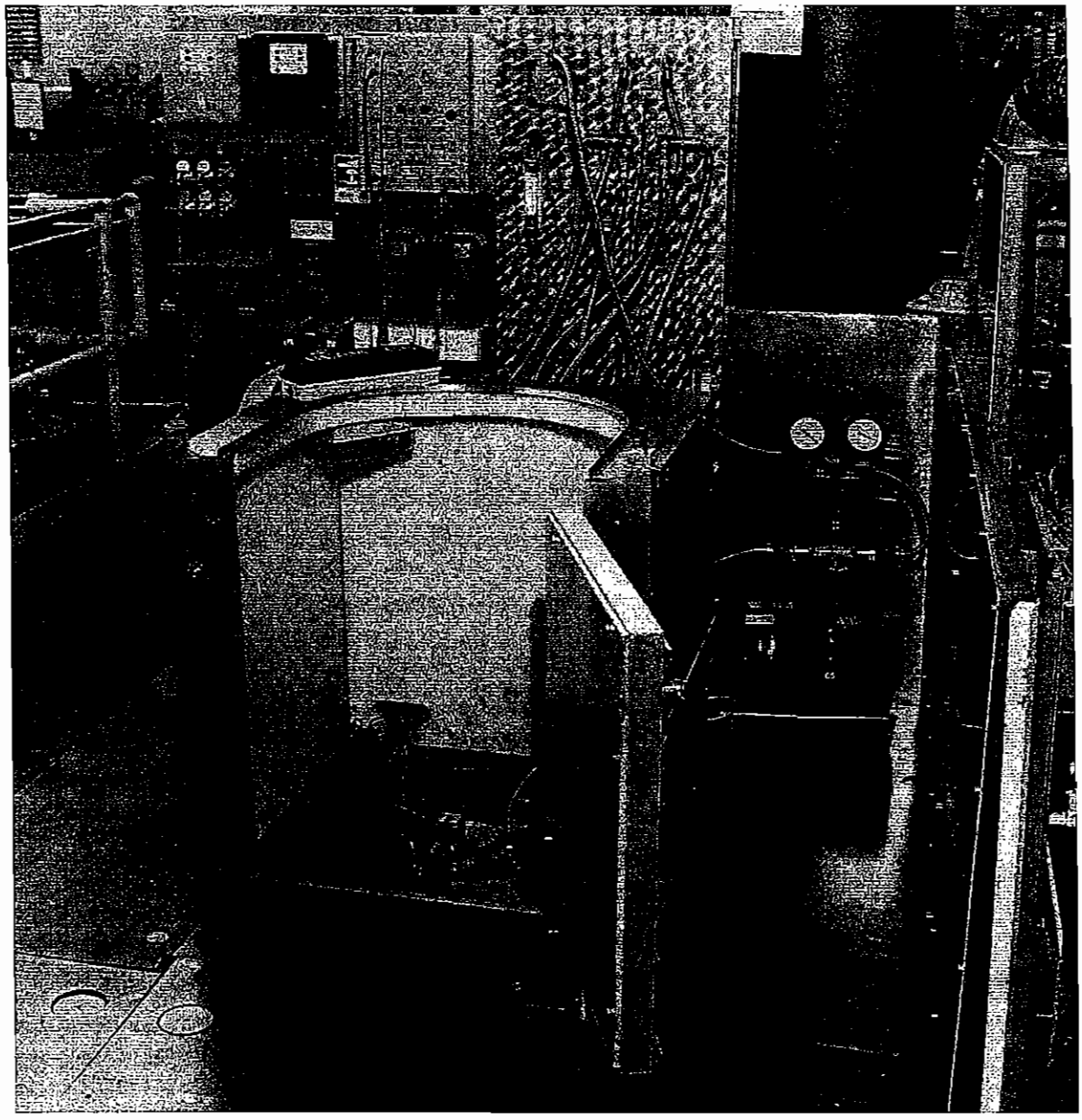


Figure 2.5: The TOSCA cloche and services panel showing the interlocks.

Access to the TOSCA CCR is via the "cloche" located on the mezzanine floor. This is interlocked by the standard ISIS key system. The interlocks on the instruments are there to try to make it impossible to get close to the neutron beam. There are two sets of interlock keys: The Master ('M') key, which is to be found on the front of the Green box and is labelled with a red tag; The remainder are 'S' keys which are located in the Blue box, see *Figure 2.6*. There are two shutter control boxes: one in the cabin and one on the services panel behind the cloche.

Note: *You only have control of the shutter if the Master key is in its Green box. If you try to operate the shutter whilst the interlocks are not complete you will trip-off ISIS.*

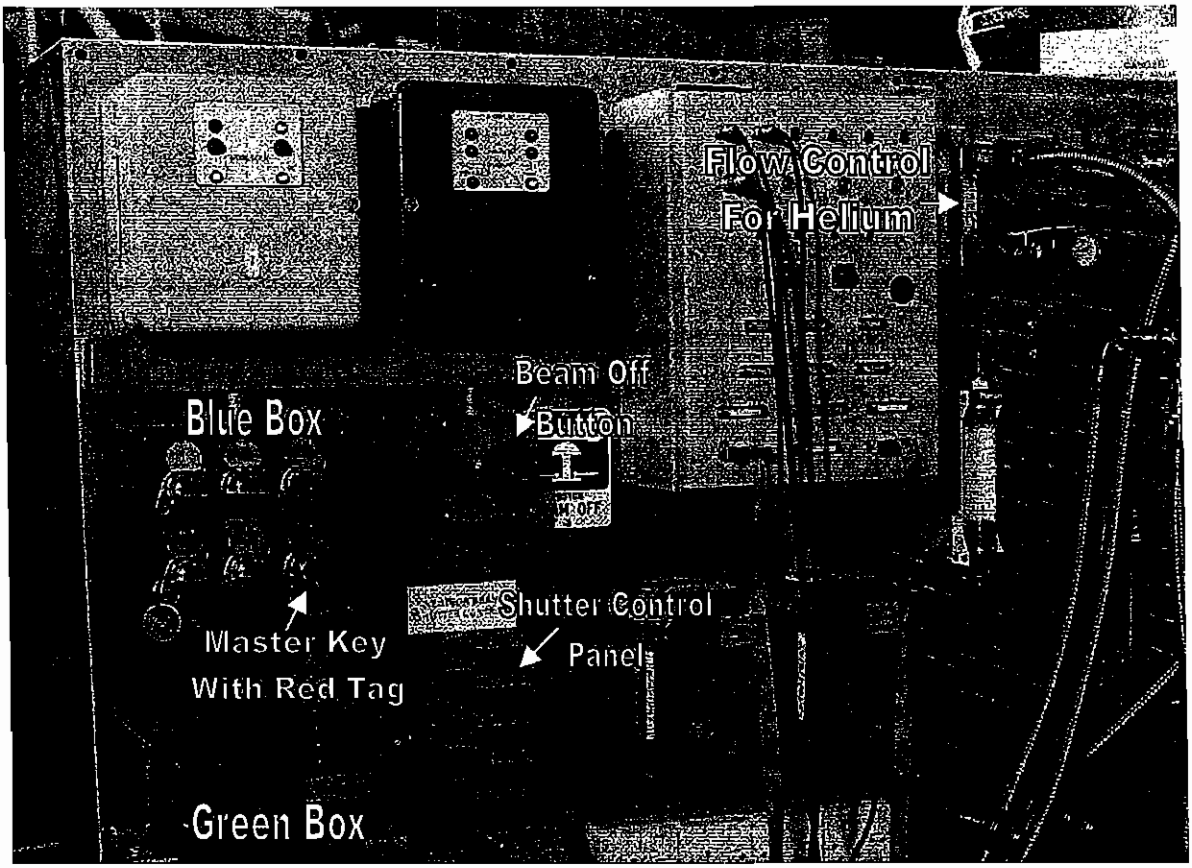


Figure 2.6: TOSCA services panel showing the Green (bottom left) and Blue (centre left) interlock boxes and the shutter control (bottom middle).

The Master key is only released when the neutron shutter is closed. Conversely the shutter can only be opened if the key is in place in the Green box.

The 'S' keys give access to the sample enclosure and other controlled areas. They can be released by placing the Master key in the bottom right hand slot of the Blue box. This is normally the only vacant slot.

Note : *The only two keys you will need to use are both on long chains.*

1. "END" the current run (the Dashboard changes to "SETUP") and write: the time, Run No and total number of microamps used into the Instrument Diary. (1 page per day.)

2. Close the shutter to the beam (green button marked "CLOSE" on the Neutron Beam Shutter Control Panel located in the cabin and also by the TOSCA enclosure, see *Figure 2.7*). The shutter takes a few minutes to close.

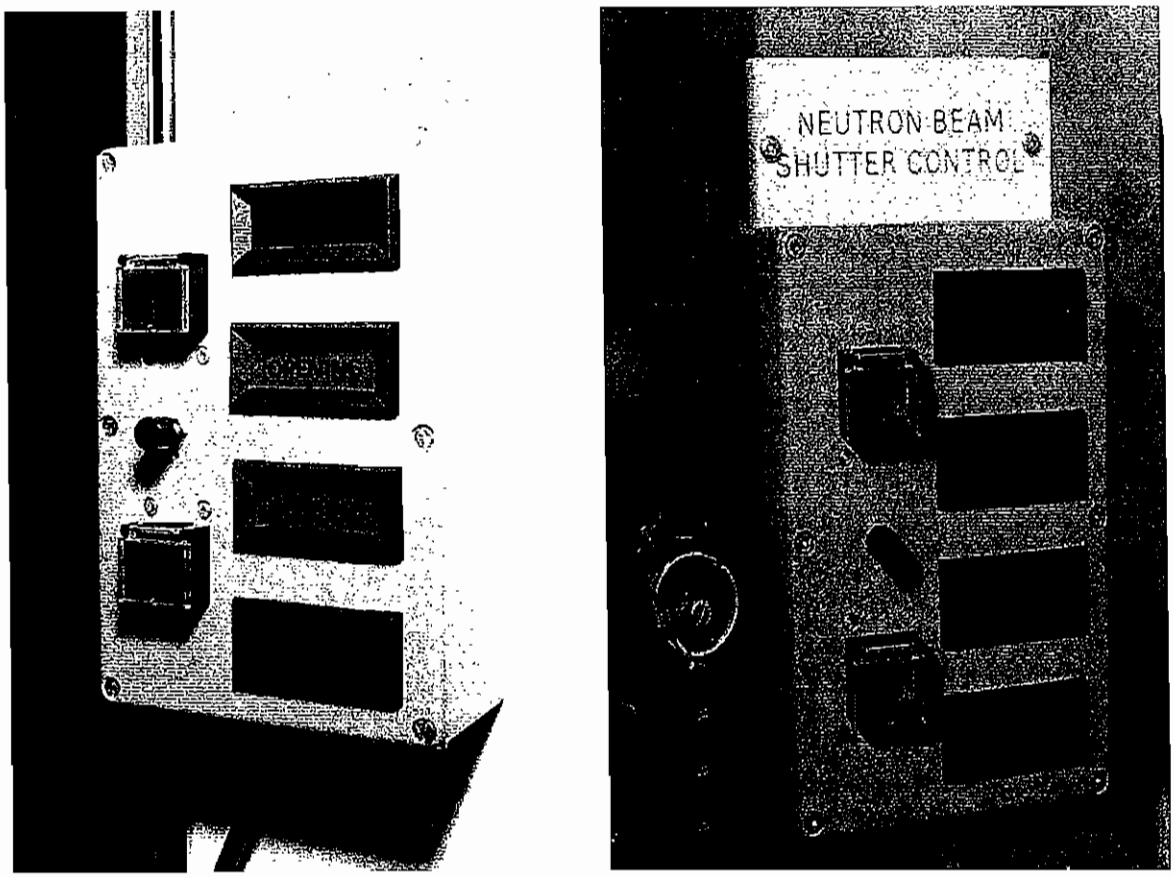


Figure 2.7: The shutter controls in the TOSCA cabin (left) and by the services panel (right).

3. Ensure the shutter is **closed.** Wait until both the blue fluorescent light, and the red "Beam On" sign are off and the green "CLOSED" light is illuminated in the shutter control panel. The radiation monitor on the wall of the target station must show a green light and a reading of less than 20 μSv/hr.
4. **Turn** anti-clockwise the "Red" (i.e. carrying a red tag) key in the "Green" box and release it.
5. Engage the Red key in the "Blue" box, and turn it clockwise.
6. This liberates all other keys in the Blue box. Locate the other chained key turn it anti-clockwise and remove it.
7. Place this key in the enclosure lock and **turn** it anti-clockwise.
8. **Rotate** the bolt fully and withdraw.
9. Open fully the valve on the flowmeter to the helium cylinder (see *Figure 2.6*). Do not adjust the regulator, the gas pressure on the gauge should read about 0.5 bar.
10. Open valve No's 1, 2 and 4 on the cryostat pump (see *Figure 2.8*) The vacuum gauges should show the pressure rising slowly, meanwhile the He gas flow is at maximum. Ensure that the light blue valve on the CCR is pointing vertically.

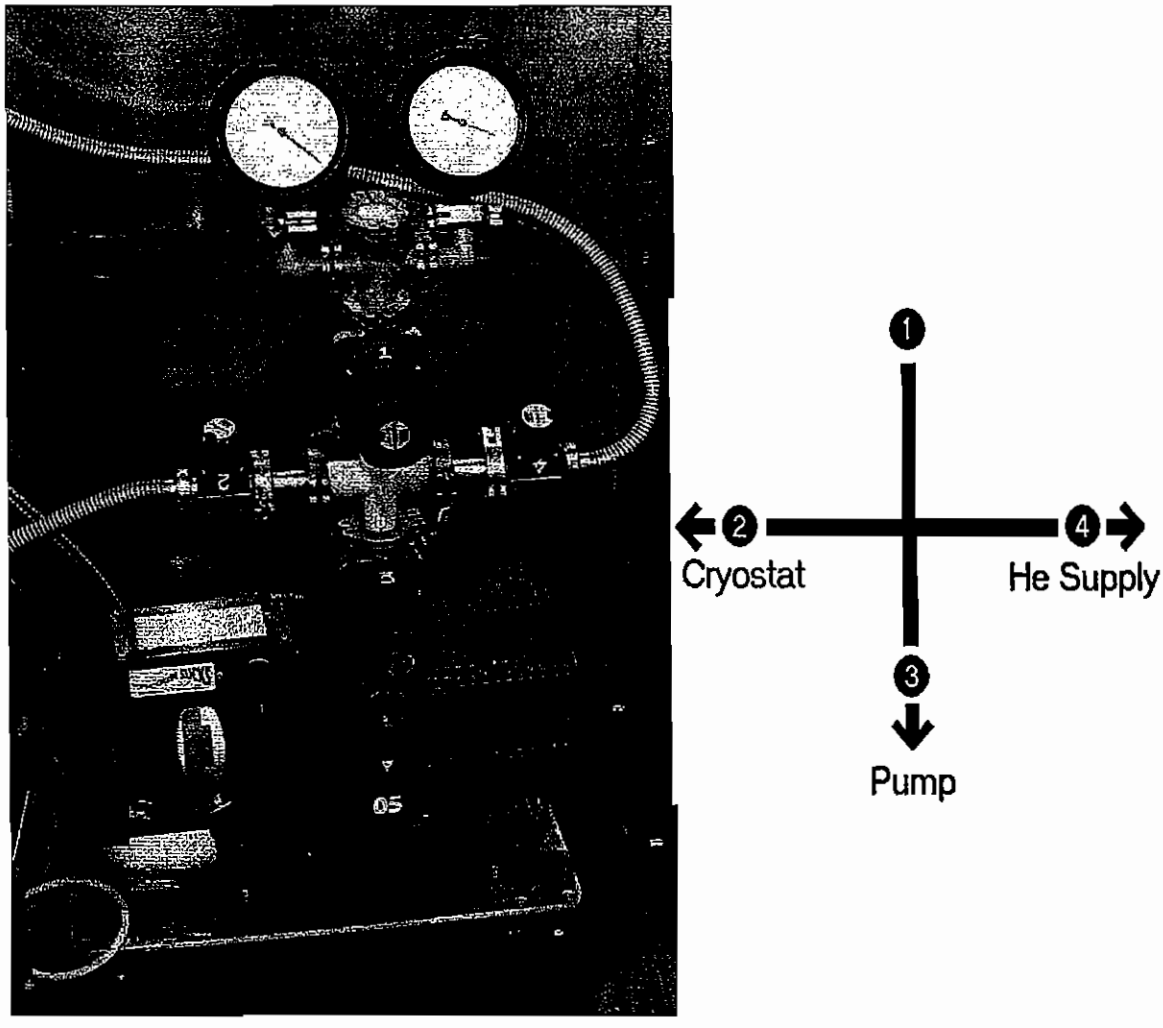


Figure 2.8: The pump manifold and sketch showing the numbering of the valves.

11. Close valve 2 when the vacuum gauge shows 1000 mbar.

Note: *Because the vacuum gauge on the cryostat pump will automatically release excess pressure: VALVE 4 MUST BE CLOSED.*

12. Remove the thermometer connection by unscrewing the knurled nut. See *Figure 2.9.*

13. Unscrew the retaining bolts at the top of the sample centrestick and withdraw the centrestick smoothly but RAPIDLY. *(Figure 2.10).*

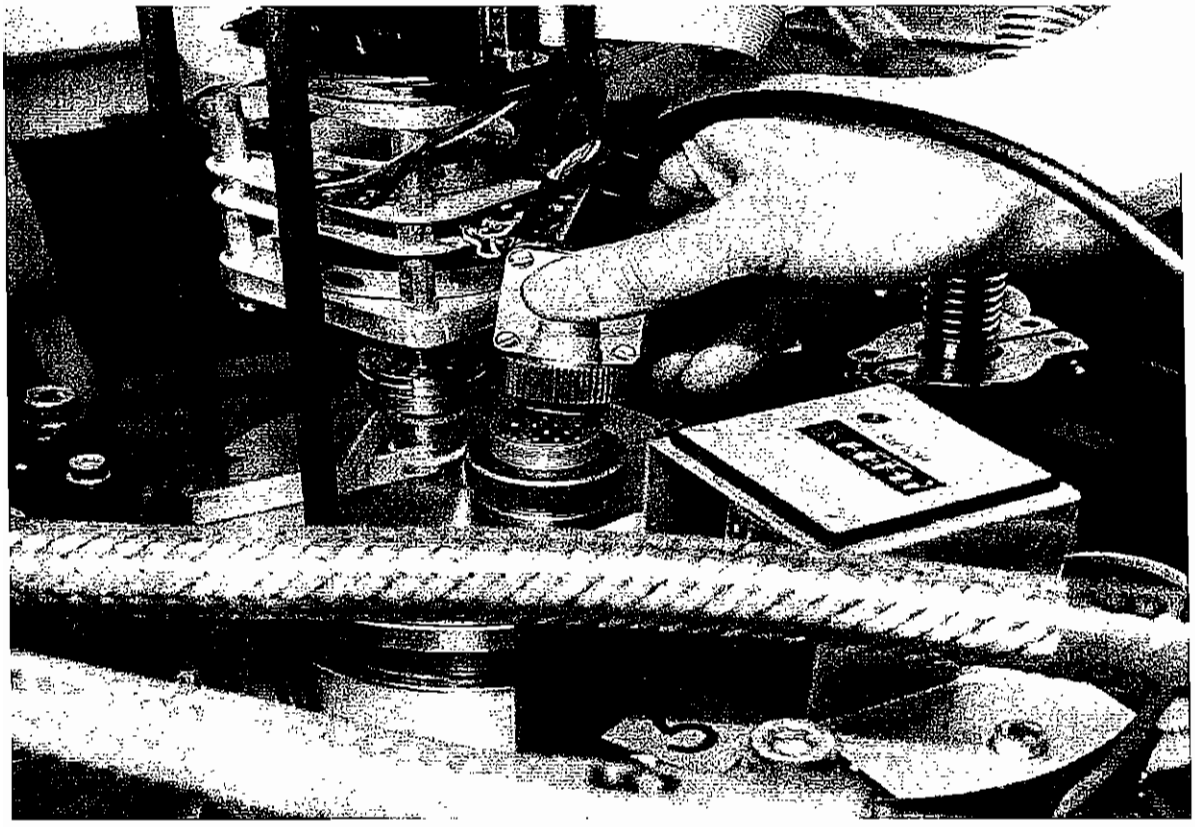


Figure 2.9: The thermometer connection on the CCR.

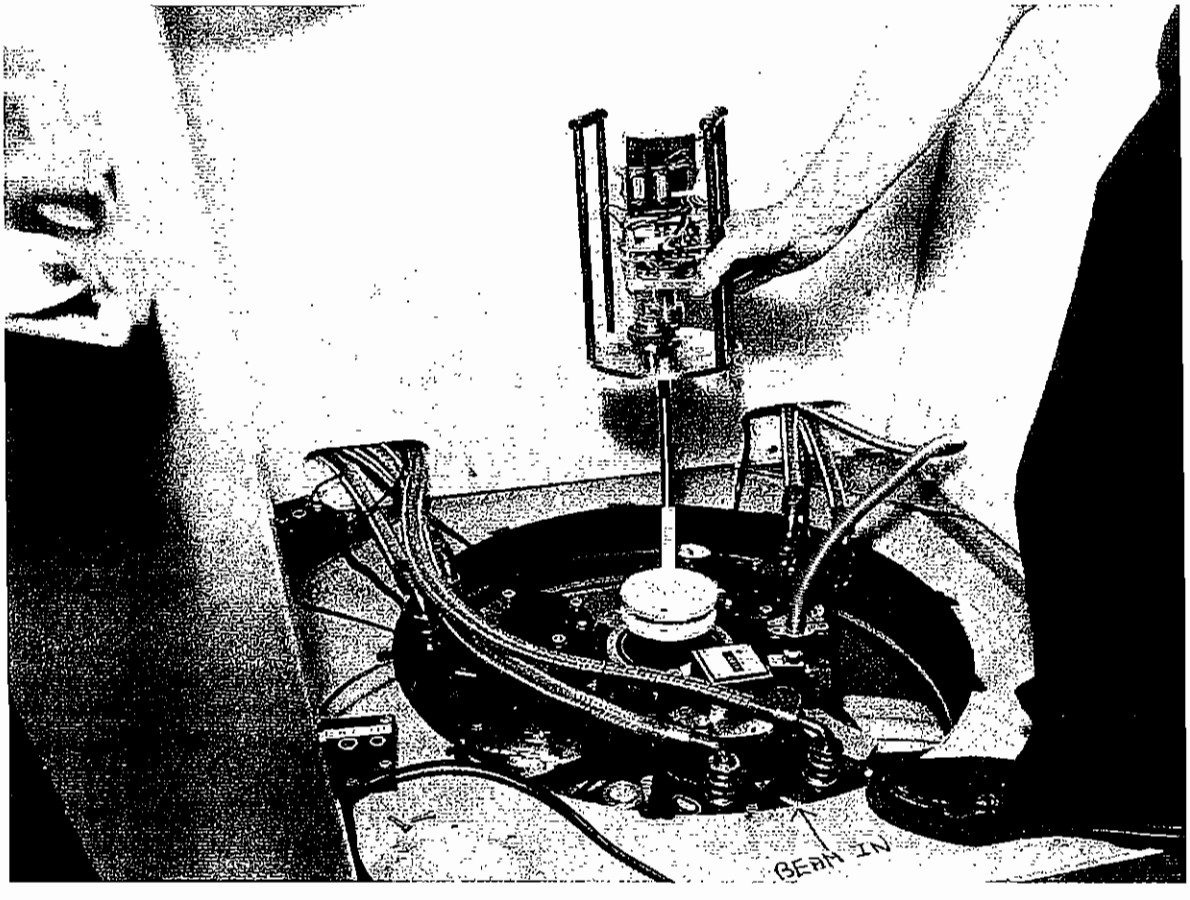


Figure 2.10: Illustrating centrestick withdrawal

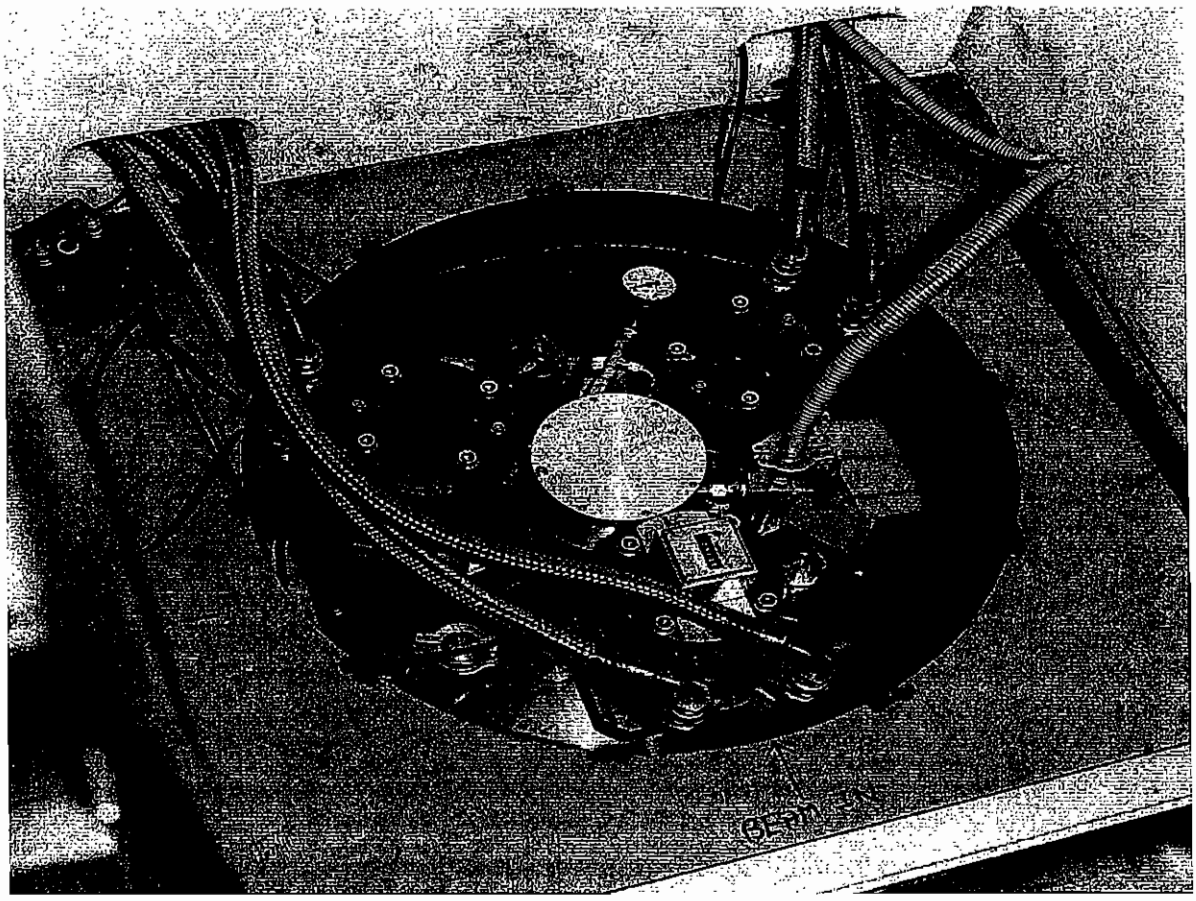


Figure 2.11: Photo graph of the cryostat with the centrestick withdrawn and blanking flange in place.

14. Cover the cryostat top with the blanking plate and bolt it down *(Figure 2.11)*.

15. Take the centrestick to the work bench and replace the old sample with new sample (see Section 2.2.)

16. Unscrew bolts retaining blanking plate, the pressure falls to 0.

17. Remove the blanking plate and push the centrestick down into the cryostat, RAPIDITY is needed but CARE must be used. Bent centresticks are expensive to replace. Ensure that the top plate is aligned so that the dowel engages in the forward hole. (Do not try to force the dowel into any other hole, it is deliberately too big to fit!!) The first sample will be facing back along the neutron beam towards the target station; the plane of the sample being perpendicular to the beam.

18. Secure centrestick lid with bolts.

19. Close valve 2.

20. Switch on the cryostat pump (switch on right hand side of pump).

21. Open valves 2 and 3, vacuum gauge begins to register.

22. WAIT until the pressure drops to 30 millibar on the gauge on top of the CCR.
23. Close all valves and switch off pump.
24. Reconnect the thermometer cable to centrestick.
25. Check which sample is oriented correctly with respect to the neutron beam.
26. Close the interlocked door (do steps 4 - 8 in reverse.)
27. Open the shutter and start collecting data (see section 4: Controlling the instrument).

2.4 Removal From Centrestick

This work should be done with the sample centrestick being on the TOSCA centrestick stand, on the work bench on the mezzanine floor.

1. Turn the hot air blower on and warm the sample.
2. Release the sample sachet from the cadmium lantern using long-nose pliers to remove the retaining wire or aluminium tape. Remember that cadmium metal strongly activates in the neutron beam.
3. Remove the sample using tweezers - or - if you must, gloved hands.

NEVER HANDLE ACTIVE SAMPLES WITH BARE HANDS.

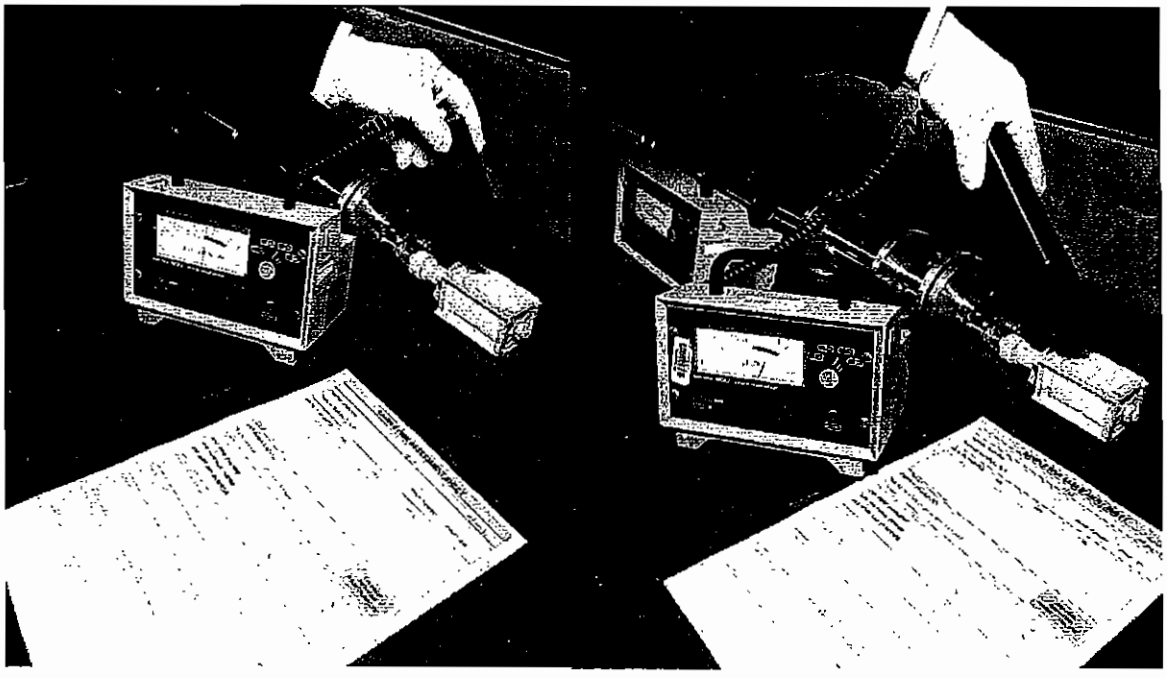


Figure 2.12: Testing the sample with β (left) and γ (right) radiation monitors.

4. MONITOR the sample with both β and γ monitors (β monitor cap off, see *Figure 2.12*). If the radiation level is less than 75 μSv consign the sample to the TOSCA active sample cupboard (se below.) If the levels are greater than 75 μSv inform the **Duty Officer** for instructions (ext: 6789)

Samples confined to the active cupboard **MUST** be in sealed plastic bags and labelled with the owner's and sample names and date. The sample environment form should also be included. Spare bags are in the tool cupboard and the prep. labs.

Note: *If you really must transfer active loose powders between sample holders or if a sachet bursts accidentally, phone the Duty Officer for instructions and help.*

NO SAMPLES MAY BE REMOVED FROM ISIS WITHOUT THE CONSENT OF HEALTH PHYSICS.

2.5 Removal of a Stuck Centrestick

Occasionally, during removal from the CCR a centrestick is found to be stuck in the cryostat. There are a number of possible causes of this, of which the most common are failure to ensure that the centrestick is dry when it goes into the cryostat, admission of air to the cryostat when the centrestick is changed or a leak around the top flange of the centrestick caused by the flange being incorrectly seated on the O-ring. By whatever means, the usual result is a small amount of air condensing between the baffles of the centrestick and the cryostat wall. In this case, warming the cryostat to 90K is sufficient to free the centrestick. If ice is present, then it is necessary to warm it to near room temperature.

THE FIRST ACTION SHOULD BE TO INFORM YOUR LOCAL CONTACT.

The sequence of actions is:

1. Fill the centrestick chamber with helium gas. ***The flange of the centrestick must be bolted down.***

2. Switch off the two CCR compressors labelled TOSCA on the ground floor by the outer wall of R55 *inside* the hall, opposite the TOSCA cabin. **DO NOT TOUCH** the five compressors that are outside the hall.

3. Warm the cryostat to 90K.

4. When the sample temperature is 90K attempt to remove the centrestick as normal (see section 2.4)

5. If the centrestick cannot be removed, wait until the cryostat has reached room temperature.

6. When the centrestick has been removed, replace the blanking flange and flush the sample volume with helium gas three times before installing the next sample.

7. Re-start the CCR compressors.

3. CONTROLLING THE INSTRUMENT

TOSCA is run by a DEC-ALPHA 500 computer located in the TOSCA cabin on the ground floor of R55. After logging-on (if necessary) the screen will look like *Figure 3.1*. In the centre of the toolbar at the bottom of the screen are four buttons labelled one to four. Each of these has its "own" screen associated with it and each screen can have as many windows as desired. The convention that is used is:

Screen 1 is used for displaying the instrument status (the "Dashboard") and controlling the instrument
Screen 2 is used to display data using GENIE
Screen 3 if for OPENGENIE
Screen 4 is for the users e.g. to telnet to their home computer.

To create a window, on the toolbar click on the icon for a terminal (4th from the left in *Figure 3.1*), a menu then pops-up and click on the item labelled DECTERM. This procedure is the same in any of the screens.

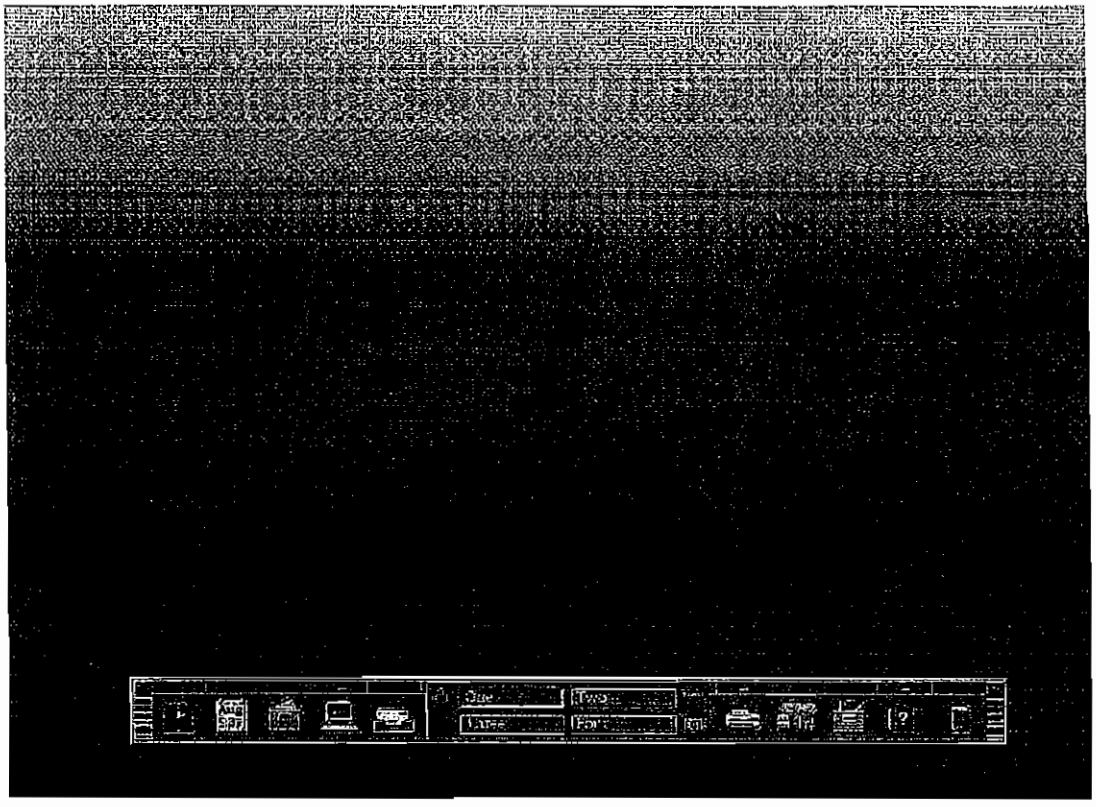


Figure 3.1: The toolbar on the TOSCA terminal in the cabin.

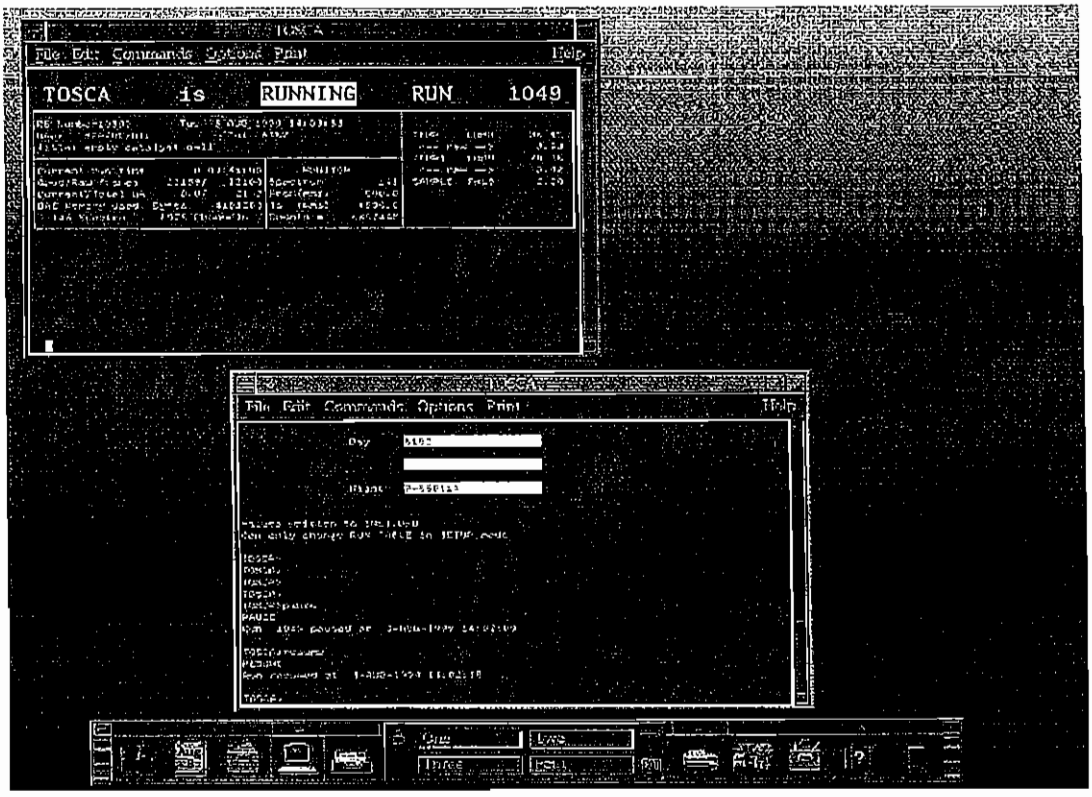


Figure 3.2: The Dashboard on the TOSCA terminal in the cabin.

For screen 1 two DECTERMs are needed. At the >> prompt type:

```
>>stat on↵
```

and the Dashboard will appear, *Figure 3.2*. The useful data in the screen are:

- The run number at the top right.
- The instrument status in the centre, this can be SETUP for changing samples, RUNNING for collecting data or WAITING for a control parameter (usually the temperature) to be true.
- The user name(s) and sample title are at the left, halfway down
- Below this is the ISIS beam current to the target and on the same line is the total microamps ("Total uA") received in the current run. For adequate statistics from a hydrogenous sample this should be at least 600 (3 - 4 hours runtime), small samples or non-hydrogenous ones will require considerably longer.
- On the right is the sample temperature ("TEMP") in Kelvin, below this is the cryostat temperature ("TEMP1" in K). If the automatic sample changer is being used then there will be an additional line with the sample position displayed.

The second window is the TOSCA control window, which should only be used for control commands such as beginning, updating and ending runs, changing temperature and starting instrument control command files. This terminal should be left in the `tosca$disk0:[tosca]` area at all times.

Note: *Do not leave files in the* `tosca$disk0:[tosca]` *area that you want to keep. The area is regularly purged.*

3.1 Change

The change command allows the user to edit the Dashboard information. Typing the command

`>> change` ↵ (can be abbreviated to `cha`)

will initiate the Dashboard editor. Move between areas using the up and down cursor keys and over type. There are six pages, you will only modify the first. This page contains title and user information. When entering the title please be informative; abbreviations or sample numbers are not very helpful. The accumulated spectra on TOSCA form a unique library whose usefulness is compromised if the spectra are not clearly identified.

To exit press `[PF1]` (found on the numeric keypad on the right of the keyboard). A prompt will appear at the top of the screen, to exit press `[e]`.

3.2 Setting Sample Environment Parameters

The top right hand portion of the Dashboard displays the sample environment parameters sample temperature (normally TEMP) and cryostat temperature (normally TEMP1). If you have changed centresticks or are using a sensor attched to the sample rather than the one built into the centrestick, you will need to input the sensor number. Each sensor is individually calibrated and a unique four digit number is written on the sensor. On each centrestick is a label with "SEN" on it that gives the sensor number. To check the censor number type:

```
FEM> cshow temp/full                                    (or temp1)
```

The computer will respond:

```
Sample environment block TEMP has flags (res,act) set

SE block name : TEMP       Requested value     5.000  Exponent              -2
Units           KELVIN     Low trip value      2.000  High trip value   30.000
Current value     17.600   Validity                T  Converted value    3.390
Run control            F   Logging                 T  Stability          0.000
Monitor period         0   Crate address           0  Crate subaddress       0
System offset      0.000   Register group          0  Preprocessor           1
Display format1            Display format2            Device number       6385
Command file               Display ?               T  Channel number         0
Secondary block SETER
```

The "Device number" is the sensor number. To input a different sensor number type:

```
FEM> cset temp/devspc=xxxx
```

Where xxxx is the sensor number.

Most spectra are recorded at the base temperature of the cryostat. If other temperatures are required, then cartridge heaters need to be attached to the sample *before* it is loaded into the cryostat. To change the sample temperature the cset command is used as follows:

```
FEM> cset temp/value=100/control
```

will set the sample temperature to 100K

Limits can be set to ensure that data are only collected between specified temperatures:

```
FEM> cset temp/value=45/lolimit=40/hilimit=50/control
```

will ensure that data is only collected while the sample temperature lies between 40K and 50K. If the sample temperature strays out of these limits the instrument will be put into "WAITING" mode.

If run control is no longer required the no control qualifier should be used

```
FEM> cset temp/nocontrol
```

When measurements are to be made at base temperature, the heater is usually switched off. If you want to warm up the sample, and there appears to be no response to the cset temp command, check that the heater is plugged in and switched on. In the TOSCA cloche, the heavy black cable must be plugged into the socket marked "HTR" on the same black box to which the temperature sensor lead is attached. The heater on/off switch is on the Eurotherm crate, in the electronics rack in the TOSCA cabin. On the back of the Eurotherm crate there is a rotary switch to set the heater voltage (Maximum voltage = 36V). The % of the maximum power is also controllable. To determine the current setting type:

```
FEM> cshow max_power/enq
```

The computer will return:

```
Value returned was    xx
```

Where xx is the % power. To change this value type:

```
FEM> cset max_power ??
```

Where ?? is the desired value ($0 \leq ?? \leq 100$)

3.3 Data Collection Commands

All the following instrument control commands may be abbreviated to three letters.

`begin`	Starts a run.
`update`	Stores the data collected so far in the current run parameter table (CRPT)
`store`	Stores the data collected up to the last update in the file `TOSCA$disk0:[tfxmgr.data]TSCA0<xxxx>.sav`. The store command should always be preceded by an update
`pause`	Pauses data collection.
`resume`	Resumes data collection.
`abort`	Aborts the current run without saving any data.
`end`	Ends the current run and stores the data in `TOSCA$disk0:[tfxmgr.data]TSC0<xxxx>.raw` The data is analysed automatically by a batch program when a run is ended. This process takes a few minutes, after that it can be viewed using GENIE.

3.4 Using Command Files

Command files are written to control the instrument. An example is:

```
$ begin                              begins run
$ waitfor 1000 uamps                 waitfor1000 µAmps
$ end                                end run
$ cset temp/value=80/lolimit=75/hilimit=85/control
                                     sets temperature limits
$ wait 00:40:00                      wait 40 mins (temperature stabilisation)
$ change title """Sample at 80K"""
                                     title change (triple "are essential)
$ begin                              begins run
$ waitfor 1000 uamps
$ end
$ exit
```

Command files are created using the VMS editor and end with the extension `.com`.

They are run from the TOSCA Control window using `@< filename>`. To interrupt a command file type [Control] Y. Note that you are unable to use the window when a com file is running.

Note:

The two commands `WAIT` and `WAITFOR` are different, and confusion over their use is one of the main causes of command file failures.

`WAIT`

This is a VMS command that waits for a specified time. The time must be given in the hrs:mm:secs format used by the VMS operating system *e.g.*

```
WAIT 01:30:00
```

will wait for one hour 30 minutes before executing the next command.

`WAITFOR`

This is an instrument control command and can be used to wait for certain amount of data to be collected. The most common usage of the command is to wait for a certain number of microamps, in this case the suffix uamps must be given after the number *e.g.* .

```
waitfor 1000 uamps
```

will wait for 1000 microamps of beam current before executing the next command. If ISIS goes off then it will sit and wait! Note that the format is rigid, there must be a space between the number and "uamps".

4. DATA ANALYSIS AND VISUALISATION.

Several programs and utilities exist to help you analyse your data including the GAUS least squares fitting program. TOSCA is unusual in that for most cases the output from the automatic analysis program is all that is required. However, if desired, the raw time-of-flight data can be analysed independently. If you are doing data analysis in your own directory make sure that you are using the TOSCA GENIEINIT .COM. Please do not log onto TOSCA and start GENIE as this seriously slows the system; use a different computer instead *e.g.* ISISA.

4.1 GENIE

GENIE is the language used at ISIS for data manipulation. A full description of which, is available in the PUNCH user manual, a copy of which resides in the TOSCA cabin. Additional copies may be obtained from the computer support office.

If you are in the TOSCA cabin the GENIE window on screen two should already be opened. If there is no GENIE window or if GENIE crashes (rare but not unknown!) it is (re)started by typing "GENIE" (upper or lower case are both OK since VMS is case insensitive) in a DECTERM window (see section 3 and *Figure 3.1* for how to start a window). This will create an additional window that can be re-sized using the mouse. By default GENIE only uses the current screen, it does not scroll off and allow you to use the scroll bar on the right of the window. This is inconvenient and can be corrected by clicking on the word "COMMANDS" at the top of the window and selecting the last item in the list "RESET TERMINAL".

If you are not in the cabin and are attempting to work on TOSCA data elsewhere, *e.g.* in the DAC, the procedure is more complicated and you should consult your local contact before starting.

When GENIE starts, a page will scroll past which includes each specialised function available and the command needed to utilise them. For reference a copy of this can be found in section 7.2. Typing the command:

```
sho sym ↵
```

will type the list.

On TOSCA, GENIE is divided into 16 workspaces, w1 – w16. The data in GENIE is completely volatile and does not alter the original data on the TOSCA disk. Thus no operation, up to and including crashing GENIE, will result in loss of data.

4.1.1 Looking at analysed files

To read in an analysed file type:

```
»r wl [tosca.user]trslxxxx.ana ↵
```

Where xxxx is the run number. To display this spectrum (stored in workspace 1) type:

»d wl ↵

This will plot the spectrum in the GENIE graphics window. The range of data displayed may be specified:

```
»d wl 50 100 0.1 0.3 ↵
```

This plots workspace 1 between 50 and 100 (x units) and 0.1 and 0.3 (y units). GENIE assumes that the two numbers following the workspace number are x values; to specify a y range, an x range must be given first.

4.1.2 Types of plot

As well as the histogram plot, it is also possible to plot the data as points, line plots or error bars. To change the type of plotting, type:

»d/l ↵	*For a line plot*
»d/h ↵	*For a histogram plot*
»d/e ↵	*For error bars*
»d/m ↵	*For the data points*

The display defaults to the last of these options entered.

4.1.3 Overlaying spectra

To overlay spectra one on top of another you can type:

```
»p w? ↵
```

Where ? is the number of the workspace to be added to the current graphics window. This is useful for comparing accurately two or more spectra. A useful

device is to display the data using the d command in a histogram format and then to overlay the error bars by using:

```
»p/e ↵
```

4.1.4 Bin sizes

The bin size represents the number of adjacent points averaged for each data point. So a binning of 1 *(i.e.* no binning) has a high accuracy, but may also have high noise levels. A numerically larger binning will give reduced noise, but the resolution will be degraded, thus binning acts as a crude type of smoothing. The advantage is that the data in the workspace is not permanently changed. To alter the binning, type:

```
»a b x ↵
```

Where x represents the binning number, usually between 1 and 10.

The GENIE command "rebin" allows different portions of the workspace to be averaged to different extents (unlike binning which operates on the whole workspace), but permanently changes the data in the workspace. Thus the best method is to copy the data to another workspace by *e.g.*:

```
»w1 = w2 ↵
```

and then to experiment on the second workspace. There are two forms to the command:

```
»reb w2 16 (2) 4000 ↵

»reb w2 16 [.02] 200 [.005] 4000 ↵
```

In form 1 with ( ) brackets the value inside the brackets is in x units. So for a spectrum in wavenumbers, the first command will rebin the data into 2 cm^{-1} intervals between 16 and 4000 cm^{-1}. Rebin truncates to the limits given. Thus if the upper limit was 2000 cm^{-1} then the data would only be retained between 16 and 2000 cm^{-1}. Note that multiple ranges are possible, as shown in the second example.

In form 2 with [ ] brackets the value inside the brackets is related to the size of the time bins in the raw time-of-flight data. When the data is transformed from time-of-flight to energy transfer a value of 0.005 is used across the entire spectrum. Thus in form 2 the spectrum is being rebinned in "4's" (0.02 = 4 x 0.005) between 16 and 200 and in "1's" between 200 and 4000 cm^{-1}. This is a particularly useful form of the command since at low energies there are many more data points than can be justified by the instrument's resolution function. Thus the data can be rebinned to improve the signal-to-noise without degrading the resolution.

4.1.5 Hard copies

To obtain a hard copy of the current data that is displayed in the GENIE graphics window, type:

```
»lpr ↵
```

A list of printers is then given and you are prompted for which printer to use (See *Table 4.1*). Just type the printer number and a postscript file will be automatically created and sent to the nominated printer.

Laser printers	**Location**
LASER 0	Computer support office, R3.
LASER 1	Coffee room, R3.
LASER 2	DAC, R55.
LASER 11	HET portacabin
LASER 14	Visitor room, R3/UG5
LASER 17	TOSCA cabin

Table 4.1: A list of the normally used printer devices.

A procedure that will always work but is somewhat more long-winded is to type:

```
»k/h ↵
```

This carries out a screen dump of the GENIE display window and creates a postscript file called DEC_POSTSCRIPT.DAT, in the directory you are currently in. To print this file from GENIE:

```
»j "plaserx dec_postscript.dat" ↵
```

Where **x** is the number of the laser printer (see table 4.1). Remember to change the disk/directory name if your file is elsewhere. These files are purged frequently so it is inadvisable to do too many at any one time.

4.1.6 Finding co-ordinates

Should you wish to find the exact co-ordinates of a peak for example you can type:

```
»c ↵
```

A 'cross-hair' will appear in the GENIE graphics window. This can be positioned using the mouse. When in the correct place click the left button and a menu will appear, select the desired option. To exit from the cursor, it is necessary to choose the "EXIT" option from the menu. By default, values and text are printed vertically at the cursor position. For annotation of a plot this is inconvenient, if

```
»c/h ↵
```

is used then the output is horizontal.

4.1.7 Useful functions in GENIE

As well as the built-in functions of GENIE, there are some routines that are specific to TOSCA that are useful to know about:

B2A

This program converts a binary file (located in a workspace) into a three column ASCII file (x, y and error) which is suitable for input to CLIMAX or to a spreadsheet. Type:

```
»b2a ↵
```

you will be prompted for the workspace, w?, and a filename. Note that b2a automatically adds .DAT to the name you give it. You are then prompted for the first and last x values (although it asks for the values in meV, it actually uses whatever the workspace x units are; cm^{-1}, Å, $Å^{-1}$).

CONVERT

This program coverts the x-axis scale from meV to wavenumbers. Type:

```
»con ↵
```

Then follow the on screen instructions.

DERIVATIVE

This calculates the derivative spectrum for a chosen workspace. Type:

```
»der ↵
```

Then follow the on screen instructions.

GAUS

This gives access to a program that performs a least-squares fit of a sum of Gaussian lineshapes to the experimental data. Type:

```
»gaus ↵
```

For more information see the FRILLS manual.

FREHACK

This is the main TOSCA data analysis program. It is normally only used if data outside the usual range (2 - 500 meV, 16 - 4000 cm^{-1}) is required or if saved (.SAV) or co-added files are to be analysed or when the batch file does not run or when the .ANA file has been corrupted and the data has to be re-analysed. (For sequential runs there is a version of REHACK called SREHACK, see next topic). Note that the . RAW file is unchanged by REHACK in any of its manifestations.

The use of a fixed final energy on TOSCA means that each energy (ω) is associated with a unique value of momentum transfer Q. A second consequence is that Q is only weakly dependent on the scattering angle, thus for the small angles subtended by the detector banks, there is no variation in Q across the detector bank. This means that the analysis of the raw time-of-flight data on TOSCA is straightforward. In essence, it consists of normalising each detector spectrum to the incident monitor spectrum, conversion to energy transfer (in meV) and summing the detectors to give a single spectrum. This process is sufficiently routine that it is carried out automatically by a batch file each time a run is ended and uses the raw time-of-flight data file (.RAW) to generate a file TRSLxxx.ANA in the directory TOSCA$DISKO:[TOSCA.USER] a few minutes later.

To run FREHACK type:

```
»frehack ↵
```

The program asks for a number of inputs. In the order in which they are required these are:

File extension:
1 for . RAW original data
2 for . SAV files saved during a run
3 for . SUM co-added data files

Run number.

Energy binning choice and a value:
1 for constant $\Delta E/E$.
2 for constant ΔE.

The raw time-of-flight data is collected in bins of equal width, thus as the energy transfer increases, there are fewer time bins in a given energy width. For most cases $\Delta E/E$ is the better choice since it better matches the resolution function of the instrument and ensures that there are sufficient data points at each energy to

correctly define the resolution. ΔE is ***not*** the resolution, it is the width ***in*** *energy* of a time bin. The required value can be calculated from:

$\Delta E/E \approx 0.0002\sqrt{E_{max}}$

where E_{max} is the highest energy (in meV) required in the spectrum. For the standard range 2 - 500 meV a value of 0.005 is appropriate. The exception to the use of ΔE/E is when it is desired to observe the elastic line, in which case ΔE should be used. The value can be calculated by re-arranging the formula to give:

$\Delta E \approx 0.0002(E_{max})^{3/2}$

The energy range to analyse.

This is usually 2 - 500 meV (16-4000 cm^{-1}). Care is needed since there is an interplay between the type and size of the energy binning and the energy range. Note that if the highest energy is too large or the value given for ΔE/E or ΔE is too small, then at some energy, there will be less than one time bin per energy element which results in a computer error.

Type of output:
1 for double differential
2 for S(Q,ω) (usual choice)
3 for both
4 for neither

Whether to exclude any detectors. Only in exceptional circumstances would this be required *e.g.* single crystal studies. For most samples the detectors are evenly illuminated, thus excluding detectors results in a reduction in signal-to-noise. If detectors are to be excluded type 1 and then either 1 (include) or 0 (exclude) for each detector in turn

REHACK then analyses the data, like QREHACK it uses workspaces w1 - w6 and puts the data in w5 at the end of the analysis. It also writes the analysed data to `tosca$disk0:[tosca.user]trslxxx.ana` so it may be read in subsequently.

Thus to analyse data using the standard conditions the series of inputs are:

```
1 ↵
1 ↵
.005 ↵          Value must be in this format, 0.005 will not work
2 ↵
500 ↵
2 ↵
2 ↵
```

LOAD_B2A

This program inputs an ASCII file to GENIE. It assumes the same format as that created by B2A i.e. first line is the title, second line is the units and then three space separated columns, x, y, error. To use it type:

```
>>load w? filename [tosca.command]load_b2a ↵
```

QREHACK

This is to have a look at the spectrum as it is being recorded. Type:

```
»qrehack ↵
```

This will result in an analysed spectrum **that is not saved.** The output of **QREHACK** is placed in workspace w5. Note that workspaces w1 - w6 are overwritten during the analysis.

SMOOTH

This creates a smoothed spectrum. The smoothed spectrum overwrites the original spectrum, for this reason you are strongly advised to copy the data to another workspace before smoothing it.

Type

```
>>smo ↵
```

The screen returns:

```
>> @TOSCA$DISK0:[TOSCA.COMMAND]SMOOGEN
>>
>>  Data smoother using Savitzky-Golay method
>>
>>    ENTER WORKSPACE:  1
```

For the workspace type the workspace number ? ***not*** w?. The screen returns:

```
>>  Workspace to be smoothed: 1
>>    SMOOTHING (%):  10
```

This controls the degree of smoothing, any integer 1-100 is usuable but 10 is a reasonable compromise between noise reduction and loss of resolution. The screen returns:

```
>>  Percentage of smoothing: 10
>>    ENTER ORDER (0, 2, 4):  4
```

This also affects the quality of the ouput. 4 works well for smoothing a background. The screen returns:

```
>>  Smoothing polynomial order: 4
>>  TR W1 TOSCA$DISK0:[TOSCA.COMMAND]SMOOGEN.EXE W1
 No OF DATA POINTS=         1109
 No OF WINDOW POINTS=          111
 POL. ORDER=             4
```

If the result is not to your liking, copy the original data to another workspace and experiment with the % smoothing and the polynomial degree until you get something you do like.

SREHACK

This program analyses spectra that were collected sequentially and co-adds the result. The co-addition is performed *before* the data is converted to energy transfer since this results in slightly better statistics. The operation is the same as for REHACK except that the user is prompted for the number of spectra and the first run number. Thus the standard inputs are:

```
1 ↵
no. of runs ↵
first run no. ↵
1 ↵
.005 ↵          Value must be in this format, 0.005 will not work
2 ↵
500 ↵
2 ↵
2 ↵
```

STRETCH

This compresses or expands the x-axis of a workspace. It is useful for comparing data of isotopically substituted molecules with the parent species. Type

```
»str ↵
```

Then follow the on screen instructions.

TEMP_PLOT and TEMP_PLOT_CURRENT

These programs plot the temperature vs time for an old run and the current run respectively. Type

```
»tp ↵
```

or

```
»tpc ↵
```

Both programs are run in the same way and are very similar. The only difference is that after starting tp you are asked for the run number and then asked to give the start date and time, whereas tpc immediately asks for the start date and time. This must be in the format:

xx-mon-year hr:min:sec

e.g.

```
12-jul-1995 09:45:00 ↵
```

The space between the year and the time is essential. You are then asked for the finish time in the same format. When prompted:

```
»Give Se block name
```

Type `temp` for the sample temperature history or `temp1` for the cryostat temperature history. You are then prompted for the temperature units (K or C) and for which log column, the default is 3 and this should be used. The program then extracts the relevant data from the temperature log. *This may take several minutes so be patient!* Eventually, it comes up with the message:

```
»Ok. Toggle mode to point plotting and d/l wl
```

"Toggle mode" switches between using the edge of data bins and the centres. Unless there are very few data points available, there is no visible difference between plots using the two modes (see "Toggle" in the GENIE manual for details). The data is stored in workspace 1 and can be treated as normal. Note that because it was generated in GENIE, it is completely volatile. It can saved as ASCII data using B2A or as binary data using the GENIE "write" command (see GENIE manual for details).

TOSCA_DIFF

In addition to the inelastic detectors there are 4 detector tubes placed symmetrically about the incoming beam *i.e.* in 180° backscattering that record diffraction patterns simultaneously with the inelastic data. The range is *0.5* - 3 in d-spacing and the resolution is $\Delta d/d \approx 3 \times 10^{-3}$. They may be analysed with **TOSCA_DIFF** the diffraction analysis program. To run, type:

```
»tosca_diff ↵
```

You will then be asked to input either the run number for a run that has ended or DAE for the current run. The output is stored in workspace 10 in GENIE. Note that a permanent file is not generated; if this is required then either B2A for an ASCII file or the GENIE command "WRITE" for a binary file that can be read by GENIE should be used (see GENIE manual for details). Uses `tosca_diff` w6 to w10 for the analysis, so data in these workspaces is overwritten.

4.1.8 Assigning files

It is occasionally necessary to look at the raw time-of-flight data from the individual detector tubes. To do this type:

```
»ass dae ↵
```

for the current run or

```
»ass xxxx ↵
```

where xxxx is the run number for a previous run. To display an individual spectrum:

```
»d s? ↵
```

where ? is the tube number. Tubes 1 - 140 are the inelastic detectors, tube 141 is the monitor and tubes 142 - 145 are the diffraction detectors. To manipulate the data it must be put into a workspace. For example, to put spectrum 3 into workspace 1, type:

```
»w1 = s3 ↵
```

Then display as described earlier.

To look at more than one tube use the multiplot command (see GENIE manual):

```
»mu s1>s56 1000 20000 ↵
```

This will display the data in detectors 1 to 56 between 1000 and 20000 μs.

4.2 OPENGENIE

OPENGENIE is the successor to GENIE. It is more flexible (e.g. unlimited number of workspaces, able to handle two-dimensional data sets, command line recall by use of up-arrow, etc...). A HELP file is available on-line on the web at http://ndbraincell/GenieReferenceManual. The advantage for TOSCA is that it enables a QREHACK to be carried out in less than a minute rather than the five minutes or so required by GENIE.

To start OPENGENIE, create a DECTERM in window 3 and then type at the TOSCA prompt:

```
TOSCA>OPENGENIE ↵
```

A series of initialisation messages are printed followed by a *caveat emptor* notice. OPENGENIE is different from GENIE in that the number of workspaces is essentially unlimited and they can be called almost anything. However, for continuity with GENIE, workspaces will be called w1 to w∞.

To look at the current run type:

```
»qrehack ↵
```

The S(Q,ω) data is placed in w5 and the double differential data in w6. To display the file type:

```
»d w5 50 100 0.1 0.3 ↵
```

A PGPLOT window is created and the data displayed in it as shown in *Figure 4.1*. Thus the display command is the same as in GENIE. The p (overlay) command is also the same.

The default x axis of the display is meV, to convert to cm^{-1} type:

```
»w? = con(w5)↵
```

where ? is any integer.

To change the binning type:

```
»a/b ?↵
```

(note difference from GENIE which is `a b ?`)

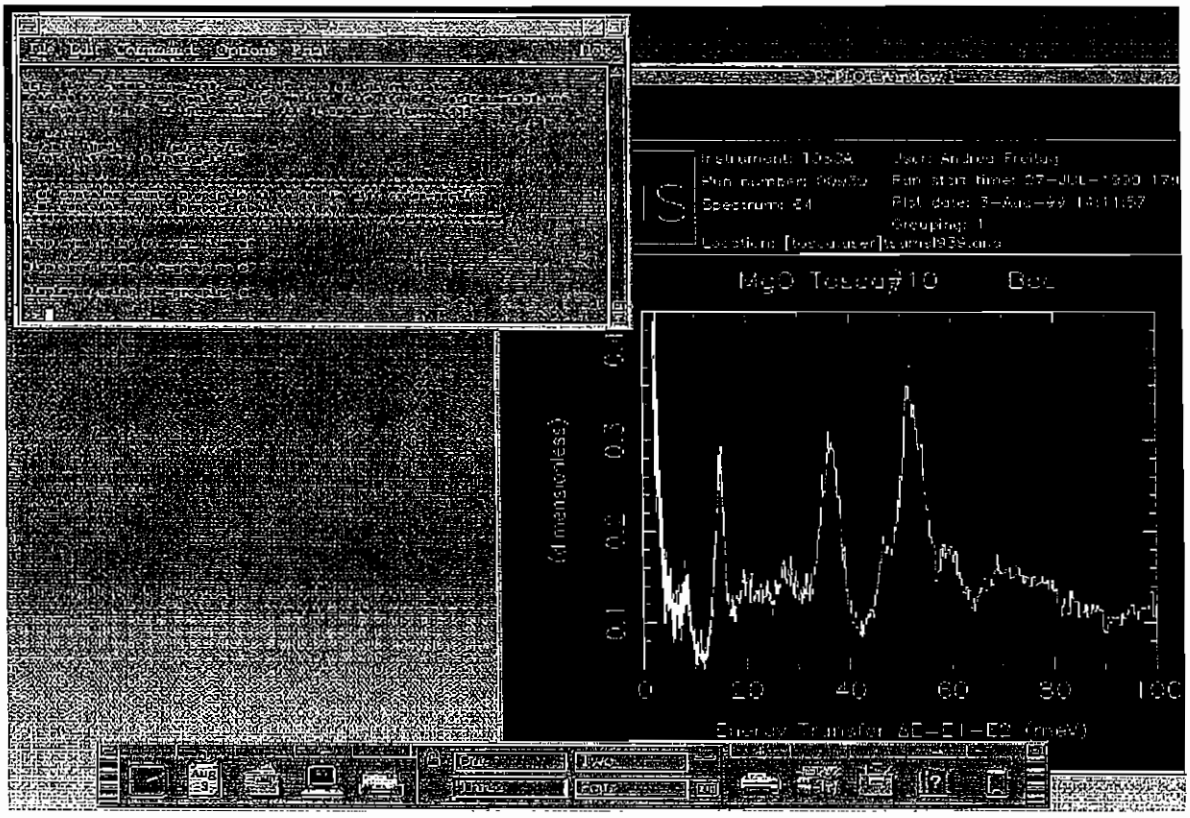


Figure 4.1: The OPENGENIE control window and display window.

To plot the spectrum the lpr command is used as in GENIE, type:

```
»lpr ↵
```

This will print the list of printers given in *Table 4.1* and ask which printer to use. Just type the printer number and a postscript file will be automatically created and sent to the nominated printer.

To look at previously analysed files type:

```
»w?=get(1,"[tosca.user]trslxxxx.ana")↵
```

`?` is any integer and `xxxx` is the run number.

To use the cursor type "cursor" at the prompt rather than just "c" as in GENIE.

Further TOSCA utilities will be added as time, enthusiasm and demand enable!

5. THE HARDWARE ON TOSCA

The purpose of this section is to supply practical information on where things are on TOSCA and how they work. It also supplies information on what the user can attempt without the risk of damaging the instrument and what should be left to the instrument scientist.

5.1 The Instrument

5.1.1 The Vacuum

TOSCA has two separate vacuum systems; the sample tank that contains the cryostat and a second vacuum system that houses the beryllium filters. Both of these are pumped with turbomolecular pumps to a cryogenic vacuum of better than 10^{-5} mbar. The sample and beryllium filter tanks on TOSCA are separated by aluminium windows.

The spectrometer vacuum pumps are located beneath the spectrometer, access is interlocked. The vacuum gauges (see *Figure 5.1*) and controls for the pumps are in the electronics cabinet on the mezzanine level in front of the TOSCA services panel on the side furthest from the target station. The upper panel is for the beryllium filter and the lower panel is for the sample environment tank. The display is in millibar. You will NOT normally touch any of this equipment, however, it is good practice to check the pressure in the two systems once or twice a day.

If the pressure is greater than 1 x 10^{-5} mbar you should inform your local contact immediately.

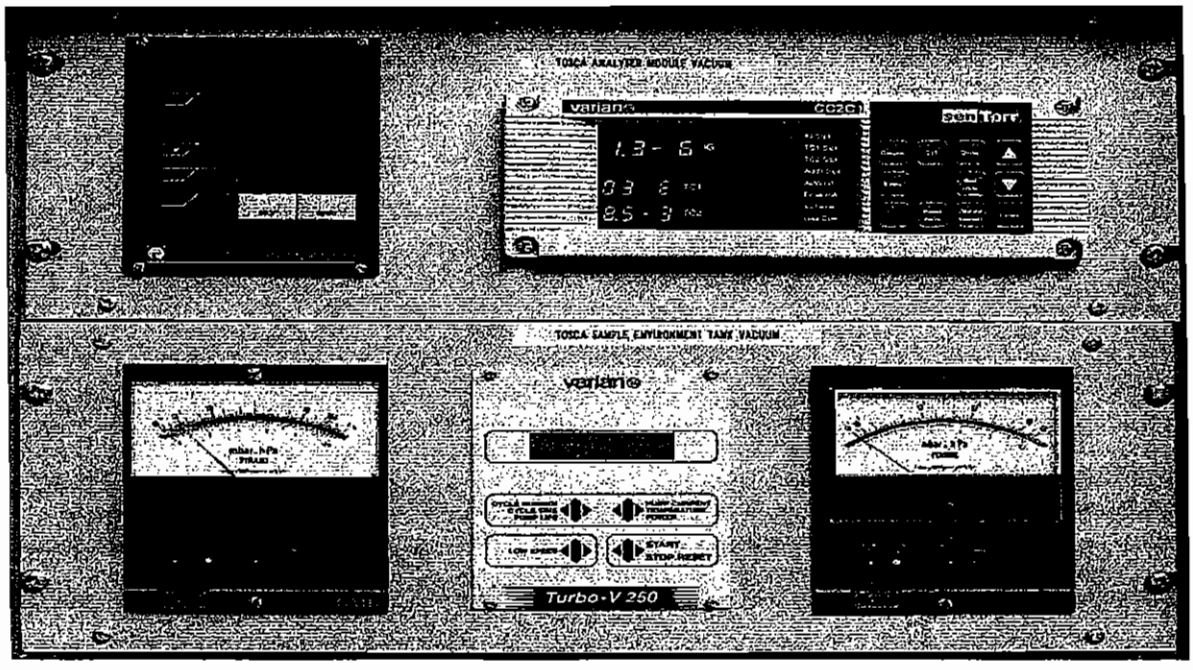


Figure 5.1. The vacuum gauges on TOSCA

5.1.2 The Beryllium Filters

The transmission of a beryllium filter is approximately doubled by cooling below ~100K. On TOSCA each Be filter is attached to a single stage CCR that cools it below 50K. The ten CCR heads are driven by five compressors that are located outside the hall, adjacent to the nearest exit from R55 (see *Figure 5.2*). The temperature of the heads is measured by Pt resistance thermometers. The output of these is displayed in the bank of ten readouts in the section of the TOSCA cabin that holds the electronics racks (see *Figure 5.3*). Each of the filters should be below 50K, there is an alarm signal (the red LED on the panel) if the temperature exceeds this. Again it is a useful precaution to check the temperatures of the Be filters once or twice a day. If a filter is above 50K check that all the compressors are operating and then inform your local contact.

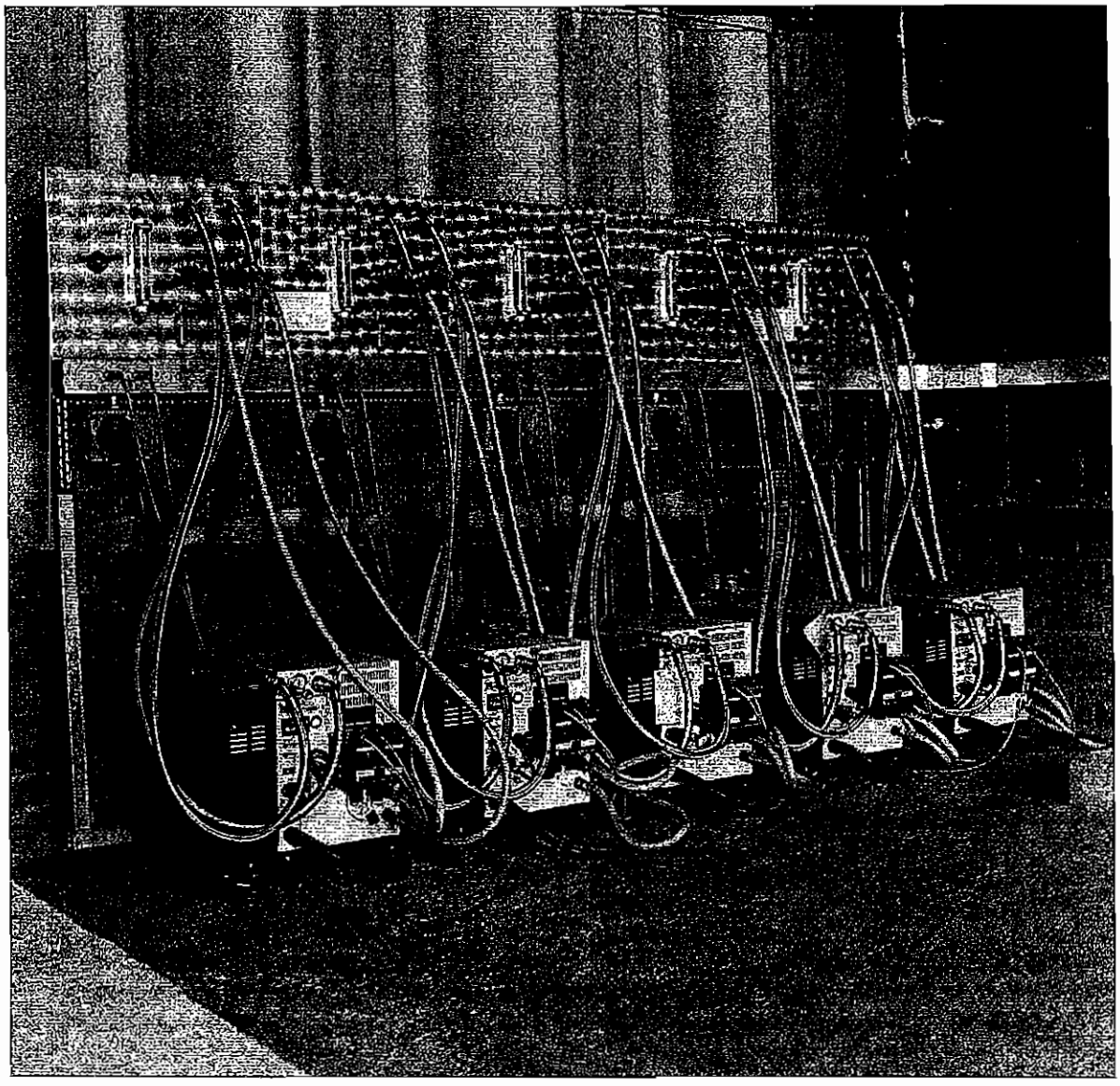


Figure 5.2: The compressors for the Be filters outside of R55.

Figure 5.3: The section of the TOSCA cabin that holds the electronics racks showing the key elements.

5.2 The Top Loading CCR

The only piece of sample environment equipment available on TOSCA is the top loading CCR. This is designed to be compatible with the standard ISIS centresticks, thus the distance from the underside of the flange to the beam centre is 1165 mm and the bore is 100 mm. The advantage of this system is that the sample can be changed without having to warm the cryostat to room temperature. It is cooled by three CCR heads, one single-stage compressor cools the outer (thermal) radiation shield to ~45K and two, two-stage heads cool the inner vacuum vessel to ~20K. The sample is cooled by helium exchange gas in this vessel. As described in section 3, the cryostat and sample temperature's are displayed on the Dashboard. The CCR heads are driven by the two compressors located inside the hall on the outer wall opposite the cabin, see *Figure 5.4*. If the sample or cryostat temperature starts to rise unexpectedly you should:

- Check whether the sample or cryostat is being heated.
- Check that there is He exchange gas in the cryostat, (there is a gauge on top of the cryostat, see *Figure 2.6*.).
- Check that both compressors are on.

If in doubt contact your local contact.

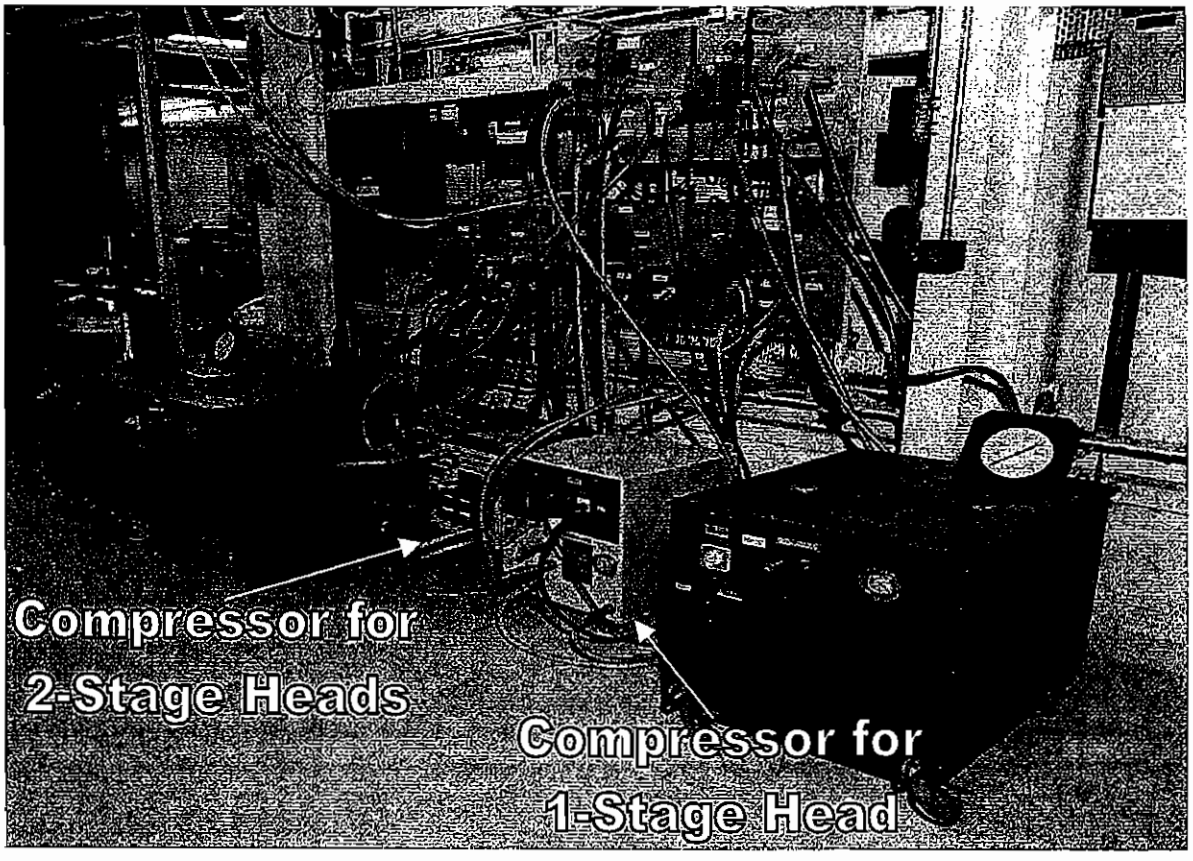


Figure 5.4: The compressors for the top loading CCR (third and fourth from the right) against the wall of R55.

6. THE VITAL STUFF

6.1. Beam off

You can check if the beam is off in a number of ways; the beam current displays at both ends of the experimental hall will read "BEAM OFF", the Dashboard display will read zero current and your data will not improve with time! You can get information on what has happened and how long the beam will be off by typing in the TOSCA Control window:

```
FEM> ISISNEWS C ↵
```

You exit by pressing "Control Y".

The beam statistics can be checked via the internet. At http://www.isis.rl.ac.uk there is a link to a page containing information about the beam status. From here graphs of the beam current can be obtained. There is a link to the MCR message board containing repair information and estimated fix times.

6.2. A Final Checklist

Before you walk out of the cabin for a quiet night in the pub, quickly go through the following checklist.

- Interlocks complete
- Shutter open
- Vacuum good
- Command file, e.g. for temperature changes, edited, stored and running

Dashboard shows "RUNNING" (or "WAITING" if using a command file).

6.3 Useful Phone Numbers

In the event of any problems with the instrument, computing or sample environment your first point of contact should be your **local contact.** If they are unavailable, then you should contact Stewart Parker, Daniele Colognesi or John Tomkinson. The home numbers can be used in the case of problems in the evening, but please not after 11 o'clock, except for dire emergencies. The Main Control room is manned at all hours and they can also be contacted if you have a problem. If you have queries about accommodation, claims or transport contact the University Liaison Office (ULS) inside working hours, ext. 5592.

To dial an office extension from outside RAL	01235 44+extension number
To make an external call from a RAL phone	9+normal number

Other useful numbers:

Emergency Fire or Ambulance	2222
Main Control Room	6789
University Liaison Office	5592

6.4 Safety Summary

Before you start your experiment please make sure that:

- You have registered with the University Liaison Office (ULS) in R3, or in the Main Control Room (MCR) if you arrive outside working hours. If you are a new user you will be issued with safety instructions, read them. You must also watch the safety video and sign the yellow card.
- You have picked up a film badge from the Health Physics Office opposite the MCR and a swipe card from the MCR.
- You have picked up and read the sample record sheet from the Data Acquisition Centre (DAC) and that you understand the sample handling instructions. This sheet is to be displayed on the instrument during the experiment.

The full safety instructions are to be found in the literature given out by the ULS. However, the salient points concerning the instrument are summarised here.

After the experiment the sample should be monitored. If the radiation is:

⇒ Greater than 75 μSv (β or γ). The ISIS duty officer (ext. 6789) must be informed to supervise the removal of the sample. Any operation concerning the sample must also be supervised by the duty officer.

⇒ Greater than 10 μSv. The sample can be removed and stored in the active sample cabinet. However, any operation that requires the sample can to be opened must be done in an active glove box.

⇒ Less than 10 μSv. The sample can be handled normally, using good laboratory practice.

After the completion of the experiment the sample can and sample should be placed in the active samples cabinet in a suitable container with a copy of the sample record sheet.

If it is necessary to transport an irradiated sample off-site, documentation must be obtained from the health physics office. Do not take the sample to them, they will come down to the instrument. Preparing the documentation will take some time so

ask for this well in advance of departure.

ISIS conforms to COSSH regulations. Any chemical process or procedure that involves chemicals, must be assessed beforehand by ISIS Safety personnel.

If you have any safety concerns ask your local contact or ring the Main Control Room.

6.5. Eating and Drinking

6.5. 1. RAL Opening Hours

R22 Restaurant

	Mon-Fri	Sat-Sun
Breakfast	7.30 - 8.30	8.00 - 9.00
Lunch	11.45-13.45	12.00-12.30
Dinner	17.30 - 19.15	18.00-19.00
Rl coffee lounge	9.00 - 15.45	Closed
R22 coffee lounge	11.30 - 13.45	Closed

These times are correct at 3/8/99. However... things can change, so beware!

6.5.2. Pubs

Blewbury	The Red Lion
Chilton	Rose & Crown
East Hendred	The Plough, Wheatsheaf
East Ilsley	The Crown and Horns, The Swan
Steventon	The Cherry Tree
Wantage	The Lamb, The Swan
West Hendred	The Hare
West Ilsley	The Harrow

7. APPENDICES

7.1 TOSCA Parameters

Moderator:	H_2O 300K (Poisoned with Gd at 2.5 cm)
Beam size at sample:	50 by 20 mm (h x w)
Beam height	1165 mm from underside of flange to centre of the beam
Detectors	140 ^{3}He proportional counters for inelastic scattering (2.5 mm effective thickness 100 mm effective length)
	4 ^{3}He diffraction detectors in backscattering
	1 incident beam monitor (scintillator)

Distances

Moderator to Sample	12.3 m
Sample to detectors	0.7 m

7.2 List of TOSCA Specific GENIE commands

```
> B2A:==@TOSCA$DISK0:[TOSCA.COMMAND]b2a
!       Converts binary files into ASCII
> CON:==@TOSCA$DISK0:[TOSCA.COMMAND]CONVERT
!       Conversion of X-scale from meV to cm-1
> DER:==@TOSCA$DISK0:[TOSCA.COMMAND]DERIVATIVE
!       Double derivative of a workspace
> FREHACK:==@TOSCA$DISK0:[TOSCA.COMMAND]FTEMP.COM
!       Conversion of tof data to energy transfer for
        15-140 detects.
> SREHACK:==@TOSCA$DISK0:[TOSCA.COMMAND]STEMP.COM
!       Conversion of tof data to energy transfer for
        15-140 detects.
> GAUS:==@TOSCA$DISK0:[TOSCA.COMMAND]NGAUS
!       Gaussian fits prog (T.Perring)
> LOADB2A:==@TOSCA$DISK0:[TOSCA.COMMAND]LOAD_B2A.COM
!       Loads 3 column (x,y,e) ASCII file
> LPR:==@TOSCA$DISK0:[TOSCA.COMMAND]LASER_PLOTS.COM
!       Screen capture and print
> QREHACK:==@TOSCA$DISK0:[TOSCA.COMMAND]QTEMP.COM
!       Conversion of tof data to energy transfer to look
        at during acquisition
> STR:==@TOSCA$DISK0:[TOSCA.COMMAND]STRETCH
!       Stretches/compresses the X scale by requested
        factor
> SMO:==@TOSCA$DISK0:[TOSCA.COMMAND]SMOOGEN
!       Smoothing using Savitzky-Golay method
> TP:==@TOSCA$DISK0:[TOSCA.COMMAND]TEMP_PLOT.COM
> TPC:==@TOSCA$DISK0:[TOSCA.COMMAND]TEMP_PLOT_CURRENT.COM
!       Temperature plotting of current or old data
> ZERO:==@TOSCA$DISK0:[TOSCA.COMMAND]ZERO_ERRORS
!       Sets all error values in a workspace to zero
```

7.3 Detector Tables

7.3.1 WIRING.DAT

NUMBER OF DETECTORS, 172, Number of Monitors 4

Index	Det	Time	Crate	Mod	Posn	Mon	Pre	Index	Det	Time	Crate	Mod	Posn	Mon	Pre
1	1	1	0	0	0	0	0	73	73	1	0	9	0	0	0
2	2	1	0	0	1	0	0	74	74	1	0	9	1	0	0
3	3	1	0	0	2	0	0	75	75	1	0	9	2	0	0
4	4	1	0	0	3	0	0	76	76	1	0	9	3	0	0
5	5	1	0	0	4	0	0	77	77	1	0	9	4	0	0
6	6	1	0	0	5	0	0	78	78	1	0	9	5	0	0
7	7	1	0	0	6	0	0	79	79	1	0	9	6	0	0
8	8	1	0	0	7	0	0	80	80	1	0	9	7	0	0
9	9	1	0	1	0	0	0	81	81	1	0	10	0	0	0
10	10	1	0	1	1	0	0	82	82	1	0	10	1	0	0
11	11	1	0	1	2	0	0	83	83	1	0	10	2	0	0
12	12	1	0	1	3	0	0	84	84	1	0	10	3	0	0
13	13	1	0	1	4	0	0	85	85	1	0	10	4	0	0
14	14	1	0	1	5	0	0	86	86	1	0	10	5	0	0
15	15	1	0	1	6	0	0	87	87	1	0	10	6	0	0
16	16	1	0	1	7	0	0	88	88	1	0	10	7	0	0
17	17	1	0	2	0	0	0	89	89	1	0	11	0	0	0
18	18	1	0	2	1	0	0	90	90	1	0	11	1	0	0
19	19	1	0	2	2	0	0	91	91	1	0	11	2	0	0
20	20	1	0	2	3	0	0	92	92	1	0	11	3	0	0
21	21	1	0	2	4	0	0	93	93	1	0	11	4	0	0
22	22	1	0	2	5	0	0	94	94	1	0	11	5	0	0
23	23	1	0	2	6	0	0	95	95	1	0	11	6	0	0
24	24	1	0	2	7	0	0	96	96	1	0	11	7	0	0
25	25	1	0	3	0	0	0	97	97	1	0	12	0	0	0
26	26	1	0	3	1	0	0	98	98	1	0	12	1	0	0
27	27	1	0	3	2	0	0	99	99	1	0	12	2	0	0
28	28	1	0	3	3	0	0	100	100	1	0	12	3	0	0
29	29	1	0	3	4	0	0	101	101	1	0	12	4	0	0
30	30	1	0	3	5	0	0	102	102	1	0	12	5	0	0
31	31	1	0	3	6	0	0	103	103	1	0	12	6	0	0
32	32	1	0	3	7	0	0	104	104	1	0	12	7	0	0
33	33	1	0	4	0	0	0	105	105	1	0	12	8	0	0
34	34	1	0	4	1	0	0	106	106	1	0	12	9	0	0
35	35	1	0	4	2	0	0	107	107	1	0	12	10	0	0
36	36	1	0	4	3	0	0	108	108	1	0	12	11	0	0
37	37	1	0	4	4	0	0	109	109	1	0	12	12	0	0
38	38	1	0	4	5	0	0	110	110	1	0	12	13	0	0
39	39	1	0	4	6	0	0	111	111	1	0	12	14	0	0
40	40	1	0	4	7	0	0	112	112	1	0	12	15	0	0
41	41	1	0	5	0	0	0	113	113	1	0	12	16	0	0
42	42	1	0	5	1	0	0	114	114	1	0	12	17	0	0
43	43	1	0	5	2	0	0	115	115	1	0	12	18	0	0
44	44	1	0	5	3	0	0	116	116	1	0	12	19	0	0
45	45	1	0	5	4	0	0	117	117	1	0	12	20	0	0
46	46	1	0	5	5	0	0	118	118	1	0	12	21	0	0
47	47	1	0	5	6	0	0	119	119	1	0	12	22	0	0
48	48	1	0	5	7	0	0	120	120	1	0	12	23	0	0
49	49	1	0	6	0	0	0	121	121	1	0	12	24	0	0
50	50	1	0	6	1	0	0	122	122	1	0	12	25	0	0
51	51	1	0	6	2	0	0	123	123	1	0	12	26	0	0
52	52	1	0	6	3	0	0	124	124	1	0	12	27	0	0
53	53	1	0	6	4	0	0	125	125	1	0	12	28	0	0
54	54	1	0	6	5	0	0	126	126	1	0	12	29	0	0
55	55	1	0	6	6	0	0	127	127	1	0	12	30	0	0
56	56	1	0	6	7	0	0	128	128	1	0	12	31	0	0
57	57	1	0	7	0	0	0	129	129	1	0	12	32	0	0
58	58	1	0	7	1	0	0	130	130	1	0	12	33	0	0
59	59	1	0	7	2	0	0	131	131	1	0	12	34	0	0
60	60	1	0	7	3	0	0	132	132	1	0	12	35	0	0
61	61	1	0	7	4	0	0	133	133	1	0	12	36	0	0
62	62	1	0	7	5	0	0	134	134	1	0	12	37	0	0
63	63	1	0	7	6	0	0	135	135	1	0	12	38	0	0
64	64	1	0	7	7	0	0	136	136	1	0	12	39	0	0
65	65	1	0	8	0	0	0	137	137	1	0	12	40	0	0
66	66	1	0	8	1	0	0	138	138	1	0	12	41	0	0
67	67	1	0	8	2	0	0	139	139	1	0	12	42	0	0
68	68	1	0	8	3	0	0	140	140	1	0	12	43	0	0
69	69	1	0	8	4	0	0	141	141	1	0	12	44	0	0
70	70	1	0	8	5	0	0	142	142	1	0	12	45	0	0
71	71	1	0	8	6	0	0	143	143	1	0	12	46	0	0
72	72	1	0	8	7	0	0	144	144	1	0	12	47	0	0

145	145	1	0	12	48	0	0
146	146	1	0	12	49	0	0
147	147	1	0	12	50	0	0
148	148	1	0	12	51	0	0
149	149	1	0	12	52	0	0
150	150	1	0	12	53	0	0
151	151	1	0	12	54	0	0
152	152	1	0	12	55	0	0
153	153	1	0	12	56	0	0
154	154	1	0	12	57	0	0
155	155	1	0	12	58	0	0
156	156	1	0	12	59	0	0
157	157	1	0	12	60	0	0
158	158	1	0	12	61	0	0
159	159	1	0	12	62	0	0
160	160	1	0	12	63	0	0
161	161	1	0	13	0	1	0
162	162	1	0	13	1	2	0
163	163	1	0	13	2	3	0
164	164	1	0	13	3	4	0
165	165	1	0	14	0	0	0
166	166	1	0	14	1	0	0
167	167	1	0	14	2	0	0
168	168	1	0	14	3	0	0
169	169	1	0	14	4	0	0
170	170	1	0	14	5	0	0
171	171	1	0	14	6	0	0
172	172	1	0	14	7	0	0

7.3.2 SPECTRA.DAT

Number of detectors 172

Detector	Spectrum	Detector	Spectrum	Detector	Spectrum	Detector	Spectrum
1	1	44	40	87	77	130	114
2	2	45	41	88	78	131	115
3	3	46	42	89	79	132	116
4	4	47	0	90	80	133	117
5	5	48	0	91	81	134	118
6	6	49	43	92	82	135	119
7	7	50	44	93	83	136	120
8	8	51	45	94	84	137	121
9	9	52	46	95	0	138	122
10	10	53	47	96	0	139	123
11	11	54	48	97	85	140	124
12	12	55	49	98	86	141	125
13	13	56	50	99	87	142	126
14	14	57	51	100	88	143	0
15	0	58	52	101	89	144	0
16	0	59	53	102	90	145	127
17	15	60	54	103	91	146	128
18	16	61	55	104	92	147	129
19	17	62	56	105	93	148	130
20	18	63	0	106	94	149	131
21	19	64	0	107	95	150	132
22	20	65	57	108	96	151	133
23	21	66	58	109	97	152	134
24	22	67	59	110	98	153	135
25	23	68	60	111	0	154	136
26	24	69	61	112	0	155	137
27	25	70	62	113	99	156	138
28	26	71	63	114	100	157	139
29	27	72	64	115	101	158	140
30	28	73	65	116	102	159	0
31	0	74	66	117	103	160	0
32	0	75	67	118	104	161	141
33	29	76	68	119	105	162	0
34	30	77	69	120	106	163	0
35	31	78	70	121	107	164	146
36	32	79	0	122	108	165	0
37	33	80	0	123	109	166	0
38	34	81	71	124	110	167	0
39	35	82	72	125	111	168	0
40	36	83	73	126	112	169	142
41	37	84	74	127	0	170	143
42	38	85	75	128	0	171	144
43	39	86	76	129	113	172	145

7.3.3 DETECTOR.DAT

Number of detectors, Number of user table parameters/detector
172, 5

Det no.	Delta	L2	Code	2theta	ut1	ut2	ut3	ut4	ut5
1	3.37	0.7450	1	90.0	4.7706	.26	.012	.66	780
2	3.37	0.7346	1	90.0	4.6635	.28	.01	.65	778
3	3.37	0.7261	1	90.0	4.5564	.3	.009	.64	780
4	3.37	0.7136	1	90.0	4.4309	.31	.008	.63	786
5	3.37	0.7025	1	90.0	4.3033	.33	.007	.62	783
6	3.37	0.6929	1	90.0	4.1826	.35	.0064	.61	784
7	3.37	0.6829	1	90.0	4.0591	.36	.0058	.60	786
8	3.37	0.6728	1	90.0	3.9446	.37	.0051	.58	790
9	3.37	0.6629	1	90.0	3.8250	.26	.012	.67	784
10	3.37	0.6531	1	90.0	3.7004	.28	.01	.66	779
11	3.37	0.6455	1	90.0	3.5964	.3	.009	.65	791
12	3.37	0.6327	1	90.0	3.4876	.31	.008	.64	777
13	3.37	0.6252	1	90.0	3.3848	.33	.007	.63	783
14	3.37	0.6176	1	90.0	3.2786	.35	.0064	.62	794
15	3.37	0.6215	1	90.0	3.2014	.3	.009	.64	780
16	3.37	0.6070	1	90.0	3.1616	.31	.008	.63	786
17	3.37	0.5904	1	90.0	2.9942	.33	.007	.62	783
18	3.37	0.6193	1	90.0	3.2218	.35	.0064	.61	784
19	3.37	0.6209	1	90.0	3.2864	.36	.0058	.60	786
20	3.37	0.6327	1	90.0	3.3935	.37	.0051	.58	790
21	3.37	0.6418	1	90.0	3.4992	.26	.012	.67	784
22	3.37	0.6484	1	90.0	3.5999	.28	.01	.66	779
23	3.37	0.6585	1	90.0	3.7035	.3	.009	.65	791
24	3.37	0.6683	1	90.0	3.8201	.31	.008	.64	777
25	3.37	0.6802	1	90.0	3.9406	.33	.007	.63	783
26	3.37	0.6897	1	90.0	4.0573	.35	.0064	.62	794
27	3.37	0.7012	1	90.0	4.1845	.36	.0058	.61	800
28	3.37	0.7133	1	90.0	4.3106	.37	.0051	.60	801
29	3.37	0.7507	2	90.0	4.8907	0.0	0.0	0.0	0.0
30	3.37	-0.860	3	177.09	0.0	0.0	0.0	0.0	0.0
31	3.37	-0.860	3	178.10	0.0	0.0	0.0	0.0	0.0
32	3.37	-0.860	0	0.0	0.0	0.0	0.0	0.0	0.0
33	3.37	-0.860	3	178.10	0.0	0.0	0.0	0.0	0.0
34	3.37	-0.860	0	0.0	0.0	0.0	0.0	0.0	0.0
35	3.37	-0.860	3	177.09	0.0	0.0	0.0	0.0	0.0
36	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
37	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
38	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
39	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
40	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
41	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
42	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
43	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
44	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
45	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
46	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
47	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
48	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
49	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
50	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
51	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
52	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
53	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
54	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
55	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
56	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
57	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
58	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
59	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
60	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
61	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
62	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
63	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
64	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
65	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
66	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
67	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
68	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
69	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
70	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
71	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
72	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
73	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
74	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
75	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
76	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0

77	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
78	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
79	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
80	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
81	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
82	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
83	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
84	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
85	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
86	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
87	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
88	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
89	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
90	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
91	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
92	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
93	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
94	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
95	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
96	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
97	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
98	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
99	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
100	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
101	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
102	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
103	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
104	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
105	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
106	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
107	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
108	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
109	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
110	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
111	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
112	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
113	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
114	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
115	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
116	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
117	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
118	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
119	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
120	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
121	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
122	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
123	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
124	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
125	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
126	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
127	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
128	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
129	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
130	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
131	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
132	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
133	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
134	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
135	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
136	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
137	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
138	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
139	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
140	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
141	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
142	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
143	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
144	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
145	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
146	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
147	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
148	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
149	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
150	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
151	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
152	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
153	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
154	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
155	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
156	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
157	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
158	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0

159	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
160	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
161	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
162	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
163	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
164	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
165	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
166	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
167	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
168	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
169	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
170	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
171	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0
172	3.37	0.960	2	0.0	0.0	0.0	0.0	0.0	0.0

7.4 Detector Voltages

LeCroy Channel	Voltage	Comment
0	0	Not used
1	1725	Inelastic detectors
2	1725	Inelastic detectors
3	1725	Inelastic detectors
4	1725	Inelastic detectors
5	1725	Inelastic detectors
6	1725	Inelastic detectors
7	1725	Inelastic detectors
8	1725	Inelastic detectors
9	1725	Inelastic detectors
10	1725	Inelastic detectors
11	0	Not used
12	850	Diffraction detectors
13	850	Diffraction detectors
14	975	Monitor

Channel 15 onwards are not used.