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The TFXA User-Guide

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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.

1. INTRODUCTION

TFXA (**T**ime **F**ocused **X**tal **A**nalyser) 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*.

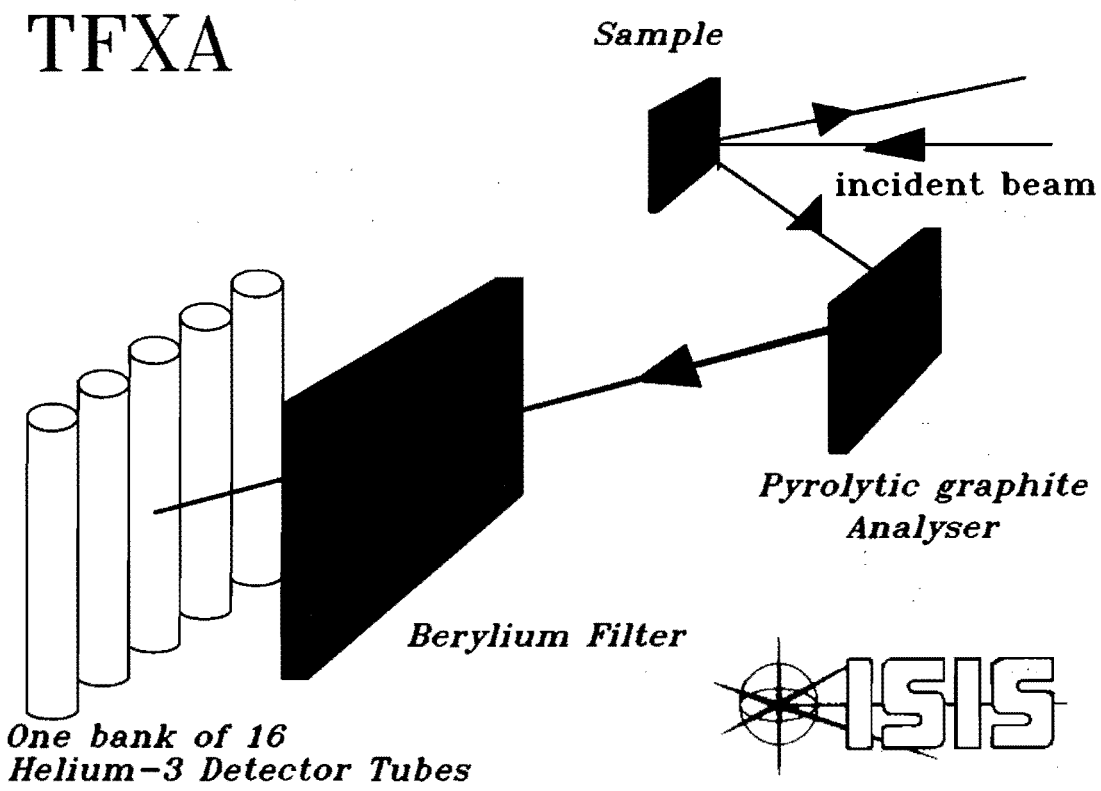


Figure 1: A schematic diagram of one half of TFXA.

The source of neutrons on TFXA 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 is the interplanar distance in the crystal, λ 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 absorbed 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 kinetic energy, E in millielectronvolts, (meV, 1 meV = 8.067 cm^{-1}), of a neutron is given by:

$$E = \frac{m v^2}{2} \tag{2}$$

where m is the mass of the neutron and v is its velocity. Rearranging (2) gives:

$$v = (2E / m)^{1/2} \tag{3}$$

and since travel time is distance/velocity 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

$$\begin{aligned} T &= t_i + t_f \\ &= \frac{L}{v_i} + \frac{l}{v_f} \\ &= L\sqrt{\frac{2E_i}{m}} + l\sqrt{\frac{2E_f}{m}} \end{aligned} \tag{4}$$

The energy transferred to the sample is

$$E_{Trans} = E_i - E_f \tag{5}$$

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 20,000 cm^{-1} (0 - 2.5eV), although the spectra are normally only analysed in the range 16 - 4000 cm^{-1} (2 - 500meV). 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 INS band 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 TFXA the design is such that there is only one value of Q for each energy, ($E_{Trans} \approx 2Q^2$). (Other instruments at ISIS *eg* HET and MARI allow both the energy and the momentum transfer to be varied). 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 frequently very different from optical spectra (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).

In addition to the inelastic detectors there are also two ^{3}He 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 *eg* 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

J Penfold and J Tomkinson, "The ISIS Time Focused Crystal Spectrometer, TFXA", RAL-82-038. This report describes the design and performance (particularly resolution) of TFXA.

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 TFXA

The vertical detector geometry on TFXA has implications for the optimal sample geometry and the design of sample environment equipment. 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) can be loaded into the cans in a glovebox.

Top Loading Closed Cycle Refrigerator

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 TFXA are cooled. Cooling below 50K makes very little difference to the spectrum, thus a Closed Cycle Refrigerator (CCR) which attains temperatures in the 20 - 30K region is adequate for most samples, see *Figure 1.1*. 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.

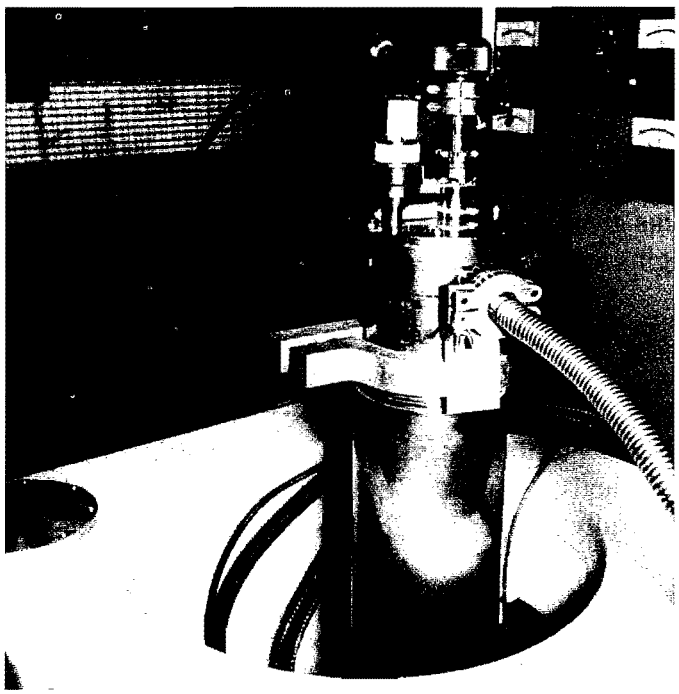


Figure 1.1: Top loading CCR on TFXA. *95RC3069*

Orange Cryostat

The orange cryostat, see *Figure 1.2*, is a conventional liquid helium cryostat and is only used when temperatures below 20K are required. Its base temperature is 1.5K (see section 3.2.2).

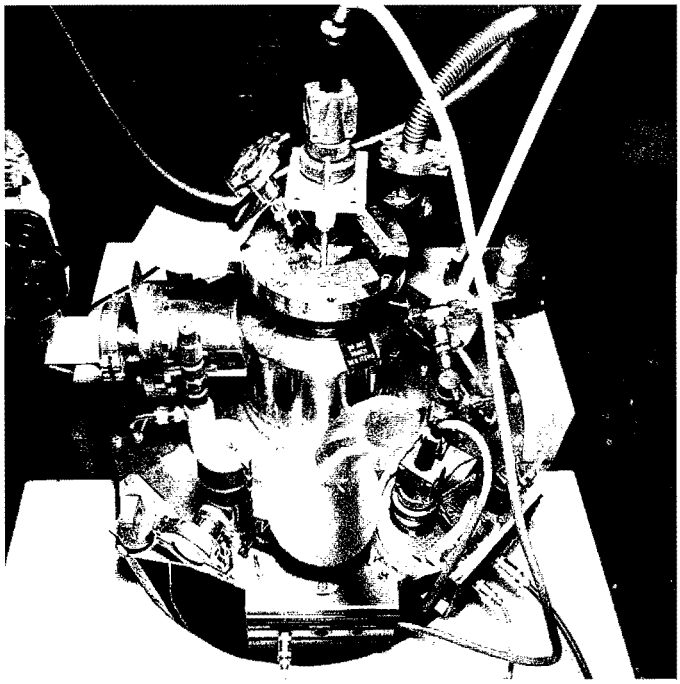


Figure 1.2: Orange Cryostat on TFXA.

McWhan Clamped Cell

The McWhan cell, see *Figure 1.3*, 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.

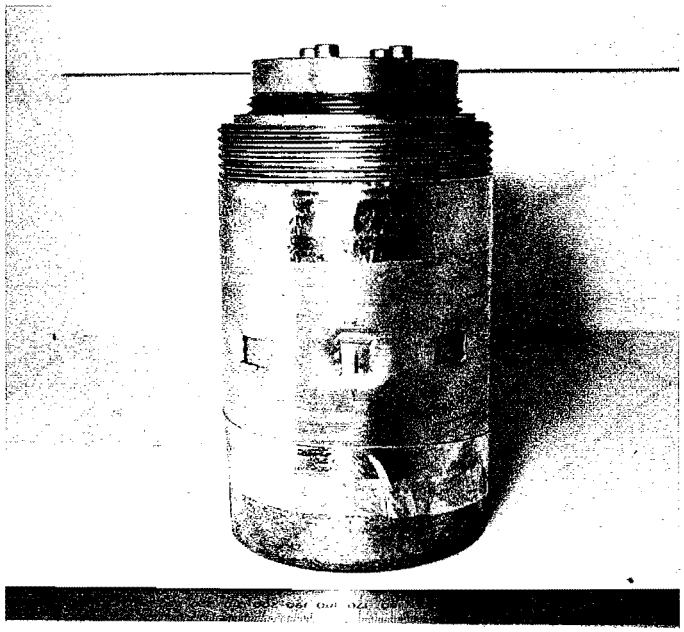


Figure 1.3: McWhan Cell *95RC3075*

2. RECORDING A SPECTRUM

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

2.1 Safety

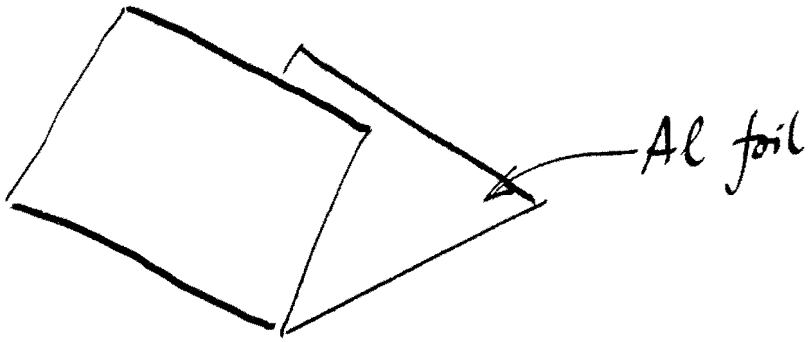
There are a number of safety issues associated with work at ISIS. The most obvious is the radiation hazard from irradiated samples and sample environment equipment. This is minimised by monitoring the radiation levels and appropriate handling and storage of irradiated materials. ***If in doubt, ask*** (your local contact, Health Physics or the Main Control Room). 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

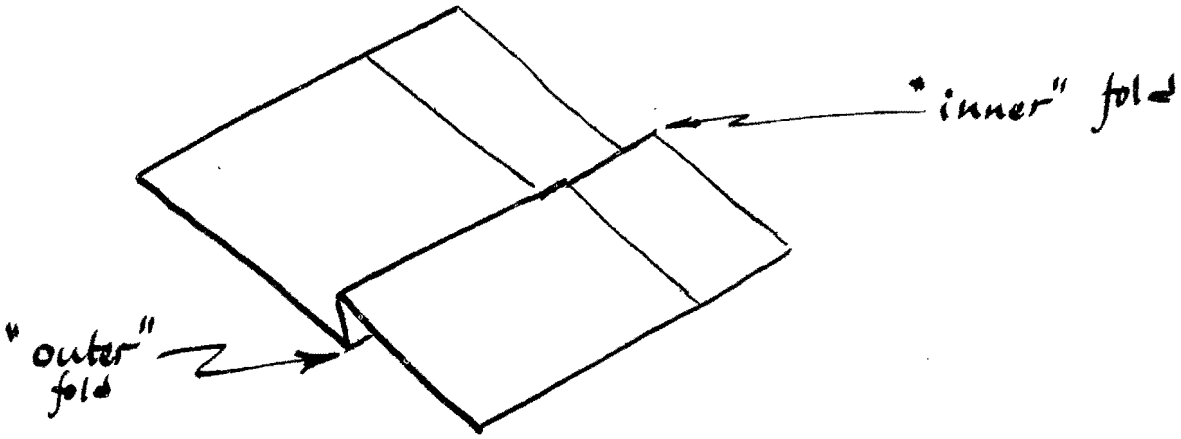
The laboratory's official handling instructions will be found on the back of the sample requirement form. You are required to observe them. For solids the easiest way to present the sample is to load it into an aluminium foil sachet. These are constructed as described in section 2.1.1. For liquids, a 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

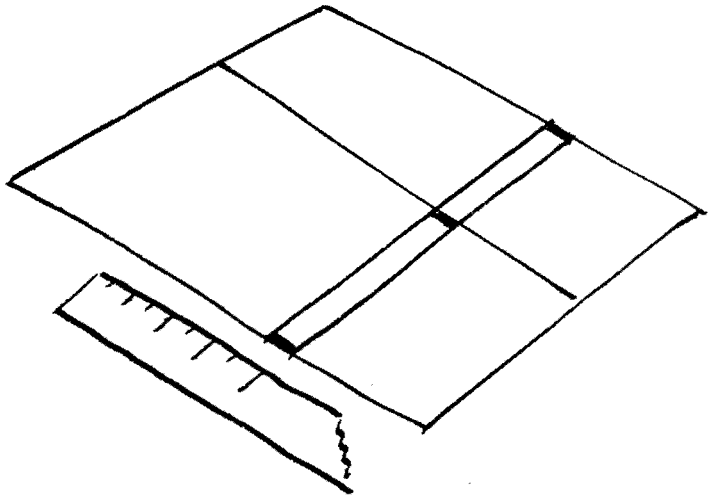


2. 1st 'Z' fold on right-hand side

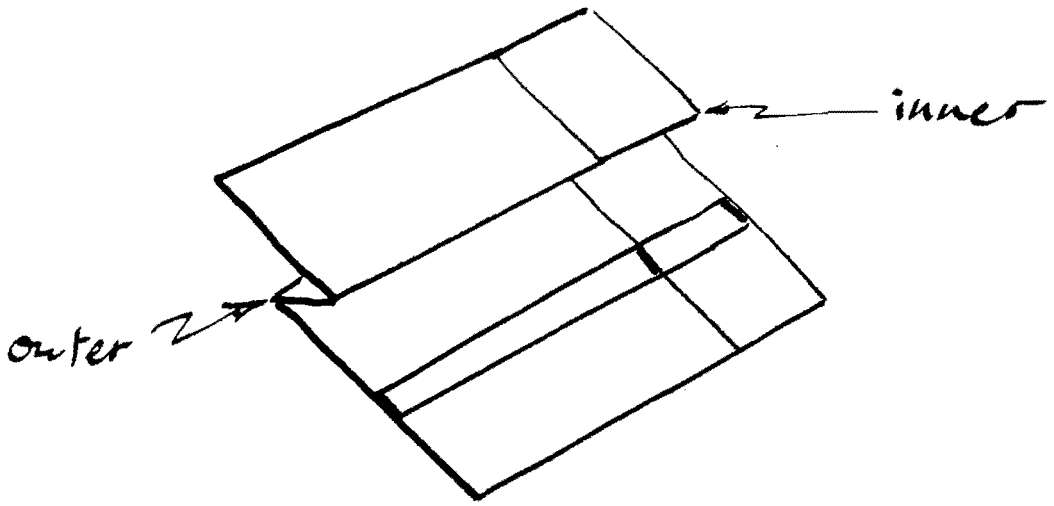


3. Press 'Z' fold flat, using back of fingernail, or plastic ruler.

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

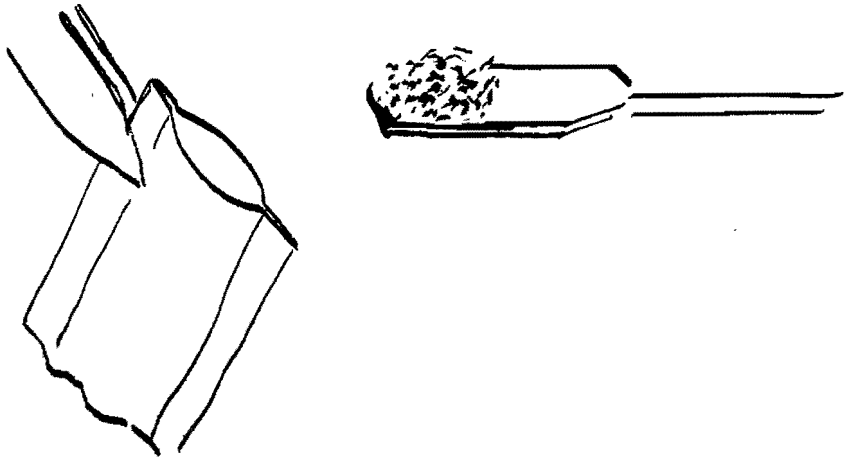


6. Press Z fold flat and cut away excess foil from the sides.

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".

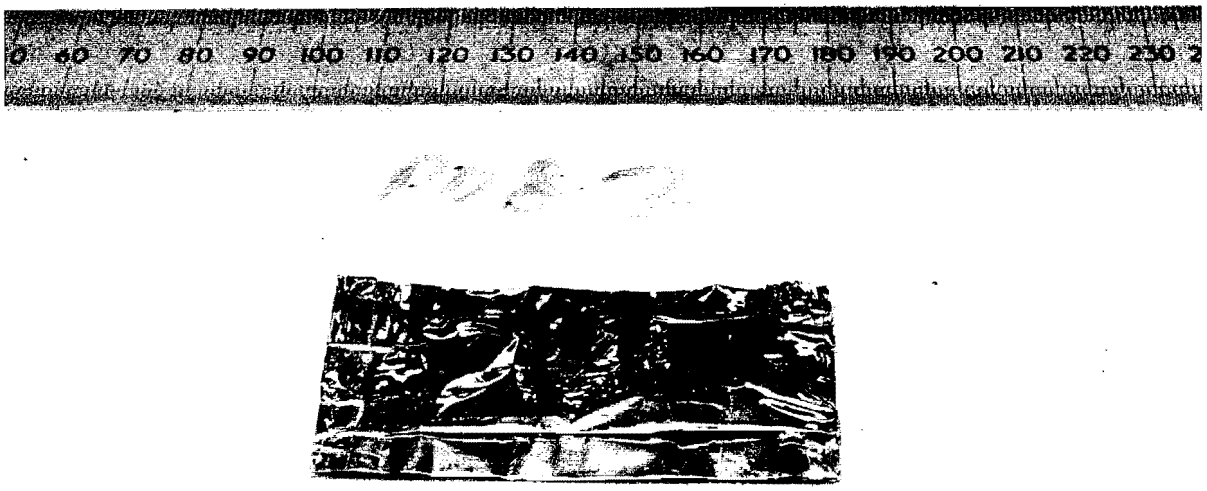


Figure 2.2.1: Picture of sachet with scale *95RC3076*

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. Enclose this sachet in some Al foil which can be gripped on the centrestick as usual.

2.2.2 Preparing an aluminium can

Figure 2.2.2 shows a 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 5mm. The can is sealed using either indium wire (narrow grooves) or with Viton O-rings (wide grooves). 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 into a sachet as normal, but the operation is carried out in a glovebox and the sachet is placed into the can before assembly in the glovebox. 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.

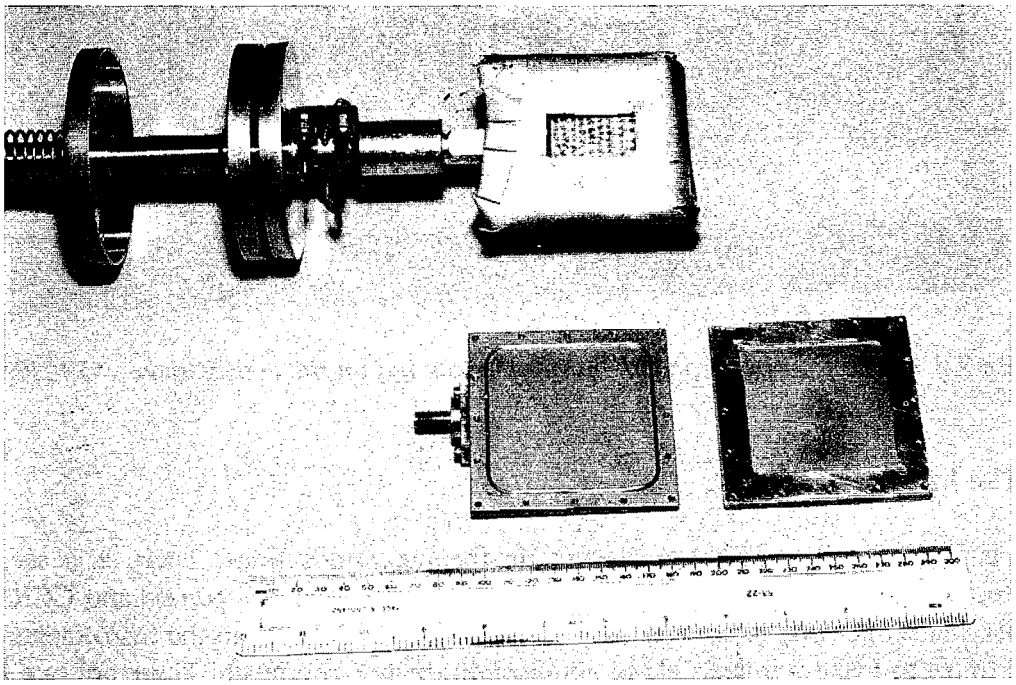


Figure 2.2.2: The components of a liquid cell and an assembled cell, shielded with cadmium mounted an a centrestick.. *95RC1026*

2.3 Loading the Centrestick

The procedure is basically the same whether the two position centrestick is used or the four-position "lantern" centrestick (*Figure 2.3.1*) is used. 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 satchet 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 two four-position centresticks, these should be used alternately 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.

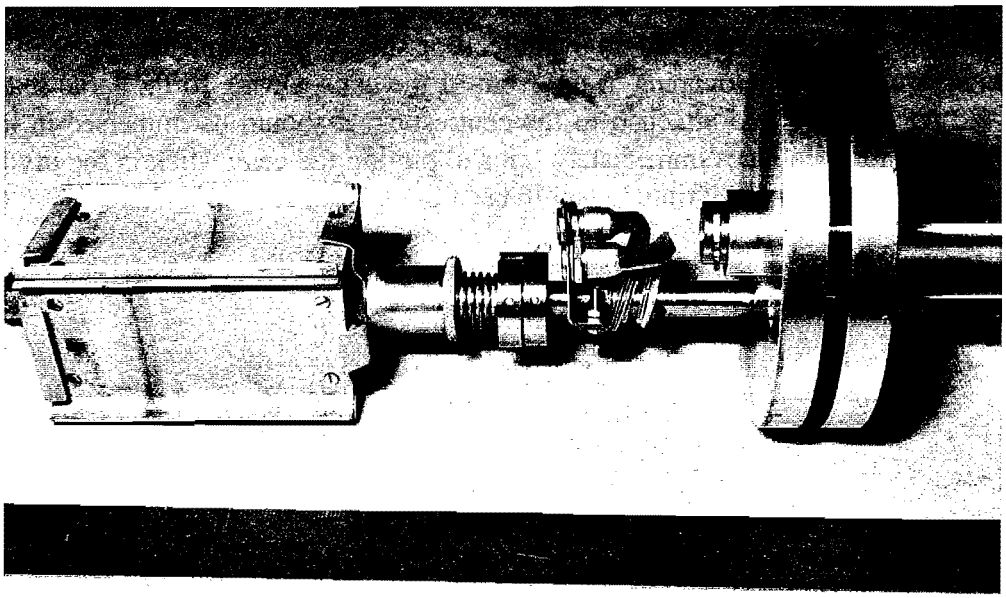


Figure 2.3.1: The four position Cd "lantern" mounted on the centrestick. 95RC3074

2.4 The Interlocked Gate

This is located at the TFXA enclosure on the mezzanine floor. There is a second interlocked area below the spectrometer containing the vacuum pumps and CCR for the beryllium filter that is not normally accessed. 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 key, which is to be found on the side of the green box and is labelled with a red tag; The remainder are 'S' keys which are located in the grey box. There are two shutter control boxes: one in the cabin and one by the telephone diagonally opposite the gate.

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

- 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 part of the Grey box.

2.4.1 Opening the Interlocked Area

Figure 2.4.1 shows the gate and interlocks to the TFXA enclosure.
Note: To "close" work backwards!

Figure 2.4.1: The TFXA gate shutter and interlocks. *95RC3066*

1. Ensure the shutter is **closed**. Wait until both the blue fluorescent light, and the red "Beam On" sign are off. The radiation monitor in the enclosure must show a green light and a reading of less than ~ 20 μSv/hr.

2. **Turn** anti-clockwise the "Red" (i.e. carrying a red tag) key in the "Green" box and release it.

3. Engage the Red key in the "Grey" box, and turn it clockwise.

4. This liberates all other keys in the Grey box. Locate the other chained key, turn it anti-clockwise and remove it.

5. Place this key in the enclosure lock and **turn** it anti-clockwise.

6. **Rotate** the bolt fully and withdraw.

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

2.5 Changing a Sample

Before changing a sample, familiarise yourself with the TFXA enclosure. *Figure 2.5.1* shows the 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.

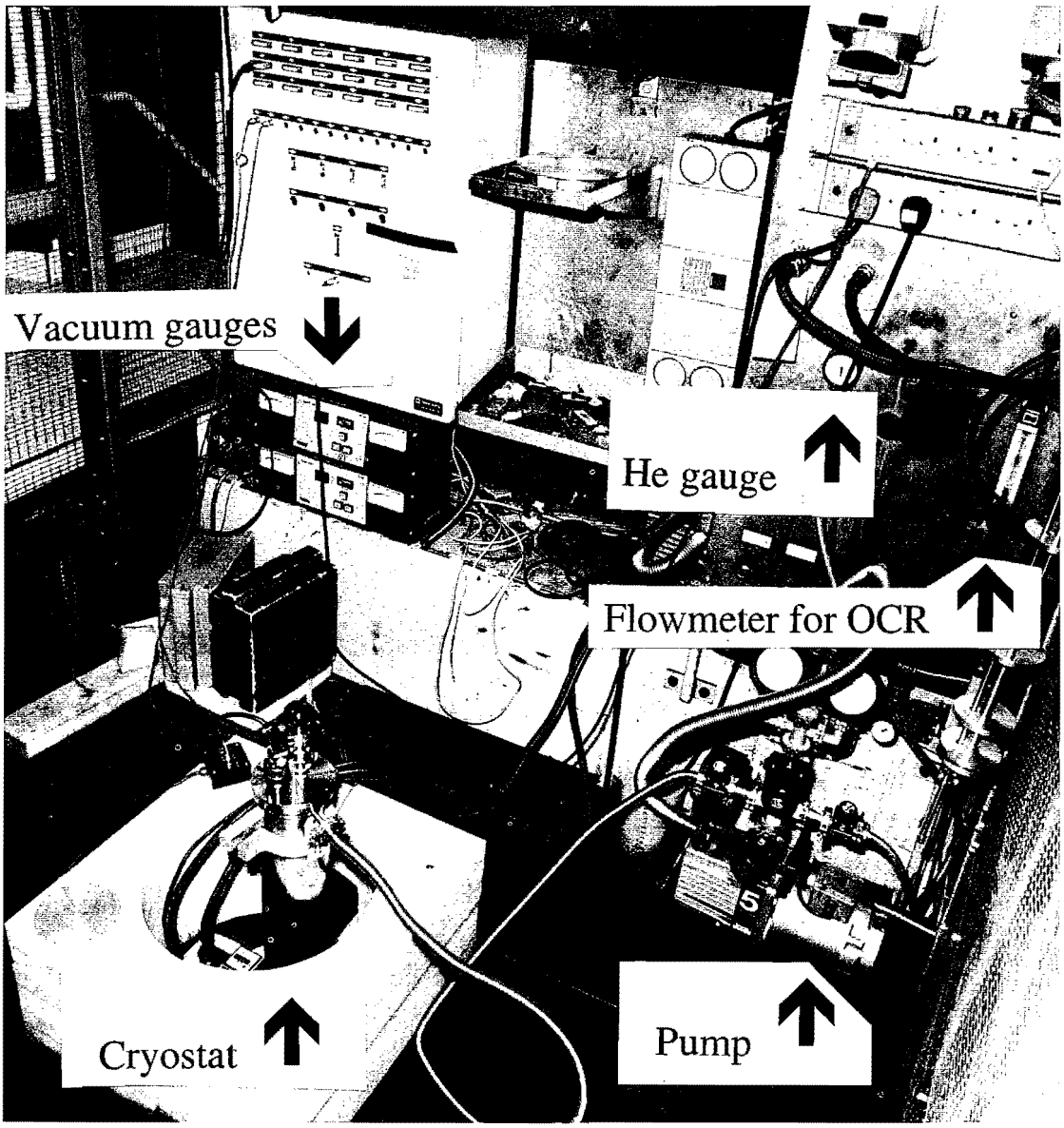


Figure 2.5.1: The TFXA enclosure viewed from the gate, *95RC3065*

1. "END" the previous 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 TFXA enclosure, see *Figure 2.5.2*). The shutter takes a minute or two to close.

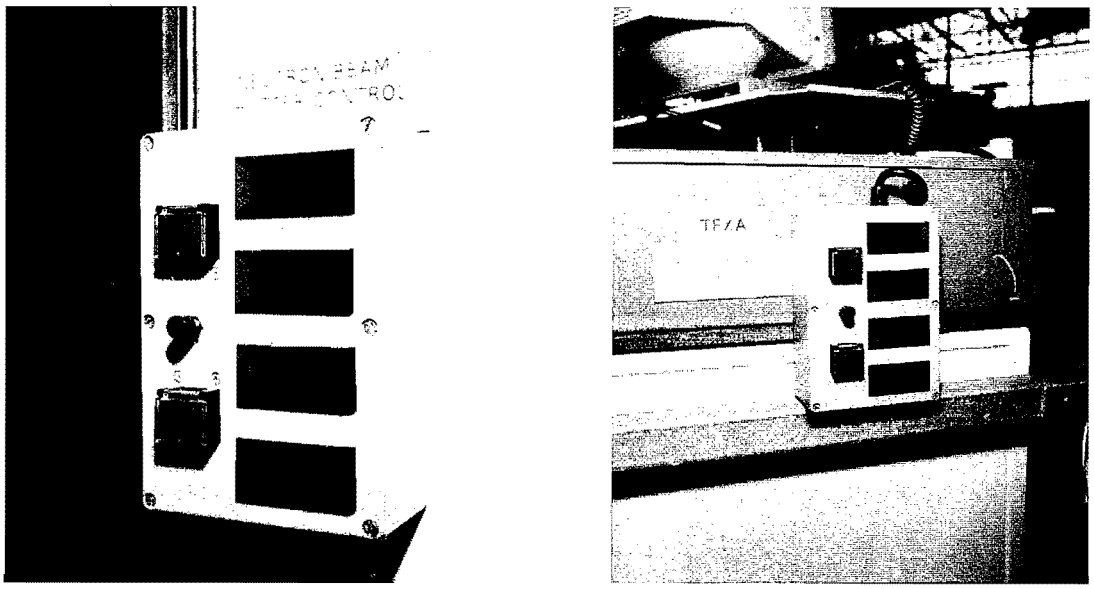


Figure 2.5.2: The shutter controls in the TFXA cabin (left) and by the enclosure (right). *95RC1012 and 95RC1011*

3. Open the Helium cylinder. This is kept below the side access stairs, operate ONLY the cylinder head valve. Do not adjust the regulator. The gas pressure on the gauge in the enclosure should read about 0.5 bar

4. Open the interlocked door (see section 2.3.1).

5. Open valve No's 1, 2 and 4 on the cryostat pump (see *Figure 2.5.3*) The vacuum gauges should show the pressure rising slowly, meanwhile the He gas pressure gauge has fallen to 0.

6. Close valve 1 when the vacuum gauge shows 1000 mbar.

Note: *Because the vacuum gauge on the cryostat pump will automatically release excess pressure : VALVE 1 MUST BE CLOSED.*

The Helium gas pressure rises to ~ 0.3 bar.

7. Remove the thermometer connection by unscrewing the knurled nut. See *Figure 2.5.4.*

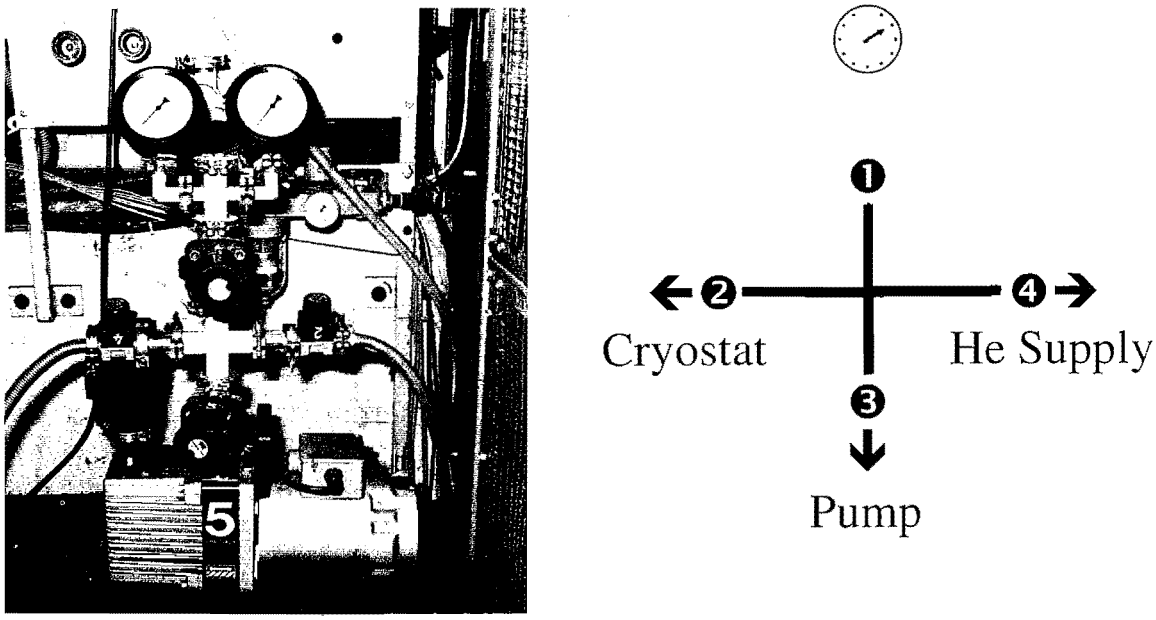


Figure 2.5.3: A photograph and sketch showing the pumping control valves. 95RC3071

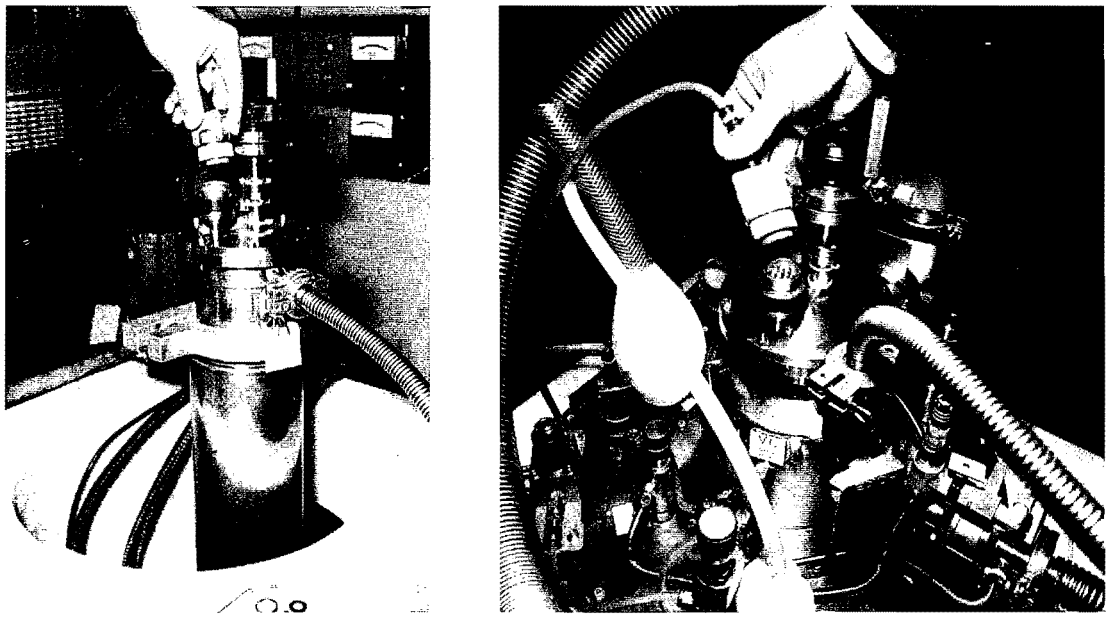


Figure 2.5.4: The thermometer connections on the CCR (left) and the orange cryostat (right). *95RC3070 and 95RC1019*

8. Unscrew the retaining bolts at the top of the sample centrestick, the gas pressure falls again to 0.

9. Withdraw the centrestick smoothly but RAPIDLY. (*Figure 2.4.5*).

10. Cover the cryostat top with a blanking plate and bolt it down (*Figure 2.5.6*); the gas pressure rises to ~ 0.3 units.

11. Close valve 4; the gas pressure rises to ~ 0.5 units.

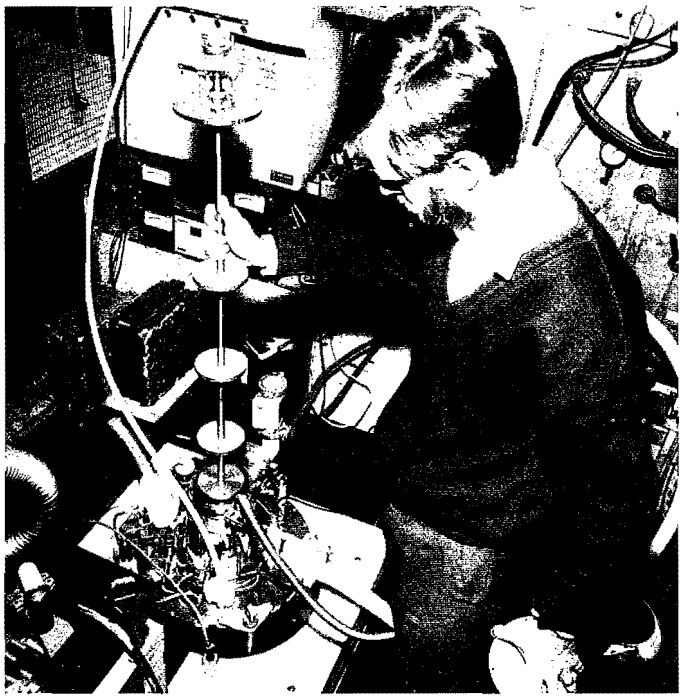


Figure 2.5.5: Illustrating centrestick withdrawal. *95RC1018*

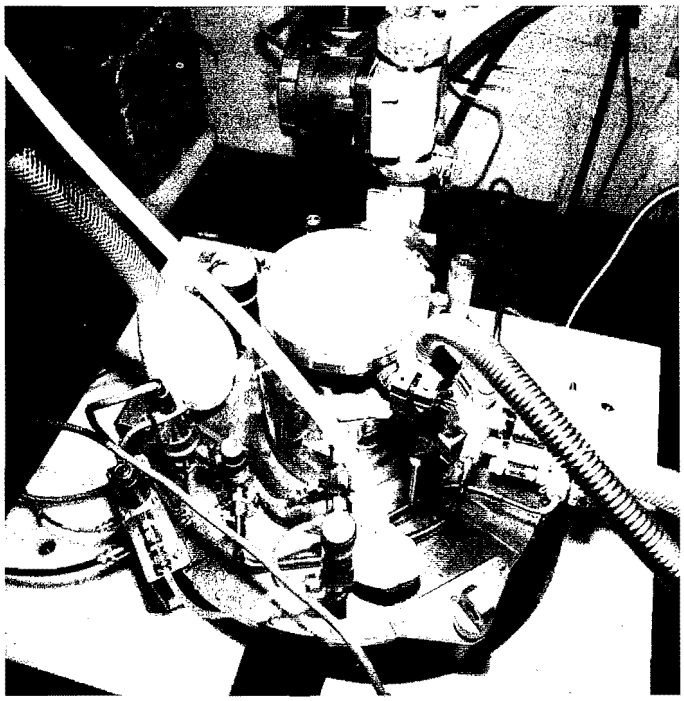


Figure 2.5.6: Photograph of the cryostat with the centrestick withdrawn and blanking flange in place. *95RC1017*

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

13. Wait 5 mins. Helium pressure must be at ~ 0.3 bar.

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

15. 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.

16. Secure centrestick lid with bolts, the pressure rises to 0.3 bar.

17. Close valve 2.

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

19. Open valves 1 and 3, the pressure rises to 0.5, vacuum gauge begins to register.

20. WAIT until the pressure drops to 20 millibar on the more sensitive gauge.

21. Close all valves and switch off pump.

22. Reconnect the thermometer cable to centrestick.

23. Check which sample is oriented correctly with respect to the neutron beam.

24. Close the interlocked door (see separate instruction.)

25. Close the Helium gas supply, at the cylinder head.

26. Open the shutter and start collecting data (see section 4. Controlling the instrument).

Note: The above instructions relate specifically to the CCR. The basic procedure (with the minor modifications given below) is the same if the orange cryostat is being used.

At step 5), before letting helium into the cryostat, the helium line should be briefly purged. After this the blue valve on the side of the cryostat should be switched to the vertical position from the horizontal.

At step 20), when the pressure in the cryostat has fallen to 20 mbar, the blue valve should be returned to the horizontal position

2.6 Removal From Centrestick

This work should be done with the sample centrestick being on the TFXA centrestick stand, on the work bench on top of 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.

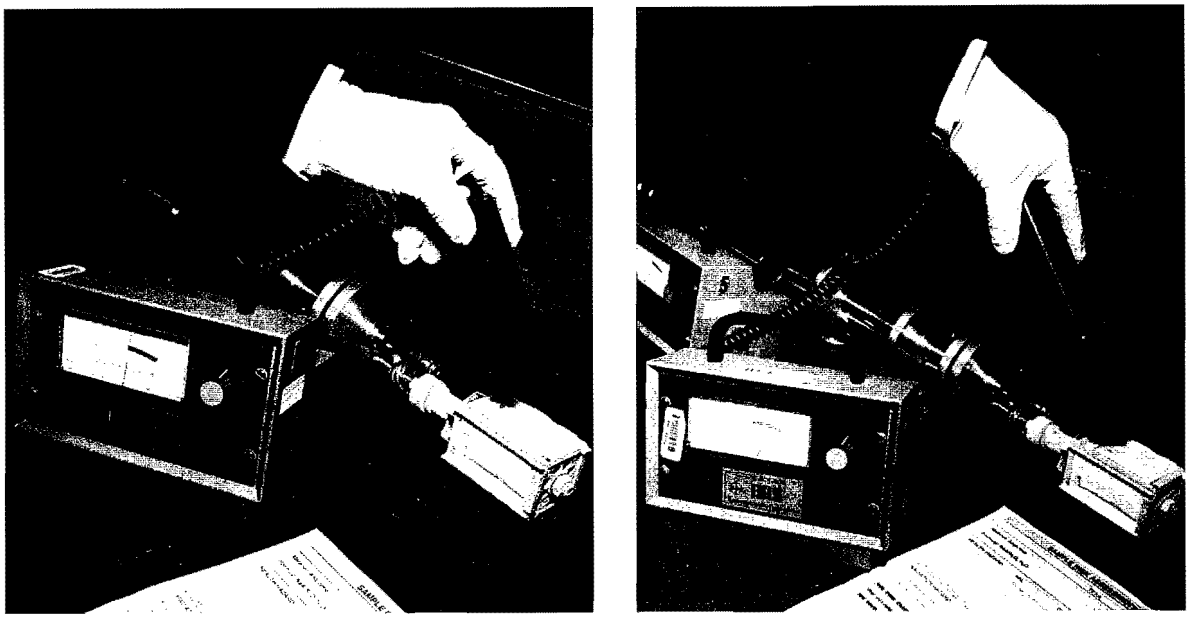


Figure 2.6.1: Testing the sample with β (left) and γ (right) radiation monitors.
95RC1008 and 95RC1009

4. MONITOR the sample with both γ and β monitors (β monitor cap off, see *Figure 2.6.1*). If the radiation level is less than 75 μSv consign the sample to the TFXA active sample cupboard (see 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.

2.7 Removal of a Stuck Centrestick

Occasionally, during removal from either the CCR or the orange cryostat, 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.
If the CCR is being used, then the sequence of actions is:

1) Fill the centrestick chamber with helium gas. ***The flange of the centrestick must be bolted down.***
2) In the TFXA enclosure, push the button marked "PUMPING UNIT" on the panel labelled SAMPLE TANK on the pumps panel, see *Figure 2.4.1* and section 3.1.1.
3) Switch off the CCR compressor labelled TFXA *and* SAMPLE on the ground floor by the outer wall of R55, opposite the TFXA cabin. **DO NOT TOUCH** the one labelled TFXA and Be FILTER.
4) On the pumps panel, wait until the "ROTATION" indicator moves to the extreme left.
5) Switch off the Penning gauge (right hand side), the Pirani gauge should begin to move a little.
6) Wait until the sample temperature is 90K and attempt to remove the centrestick as normal (see section 2.4)
7) If the centrestick cannot be removed, wait until the cryostat has reached room temperature.
8) 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.
9) Re-start the pumps by pushing the "PUMPING UNIT" button. When the pressure has fallen to 10^{-4} mbar, re-start the CCR compressor.

If the orange cryostat is being used, then the sequence of actions is:

1) Fill the centrestick chamber with helium gas. ***The flange of the centrestick must be bolted down.***
2) Reduce the helium flow on the cryostat to almost zero.
3) Heat the cryostat using the internal heaters.
4) Wait until the sample temperature is 90K and 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) Increase the helium flow to its usual level (4 - 6 l/min).

3. THE HARDWARE ON TFXA

The purpose of this section is to supply practical information on where things are on TFXA 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.

3.1 The Instrument

3.1.1 The Vacuum

TFXA has two separate vacuum systems; the sample tank that contains the sample environment (usually a cryostat) and a second vacuum vessel that holds the beryllium filter. Both of these are pumped with turbomolecular pumps to a cryogenic vacuum of 10^{-6} mbar. The sample and beryllium filter tanks on TFXA are separated by an aluminium window. To change sample environment equipment it is necessary to bring the sample environment tank up to atmosphere. *This is a task that must be done by the local contact or instrument scientist.*

The main spectrometer vacuum pumps are located beneath the spectrometer, access is interlocked. The vacuum gauges (see *Figure 3.1.1*) and controls for the pumps are in the TFXA enclosure. The upper panel is for the beryllium filter and the lower panel is for the sample environment tank. The display is in millibar. There are push button controls for the pumps and to start pumping it is only necessary to press the 'PUMPING UNIT" button.

You will **NOT** normally touch any of this equipment, however you should check that all is working.

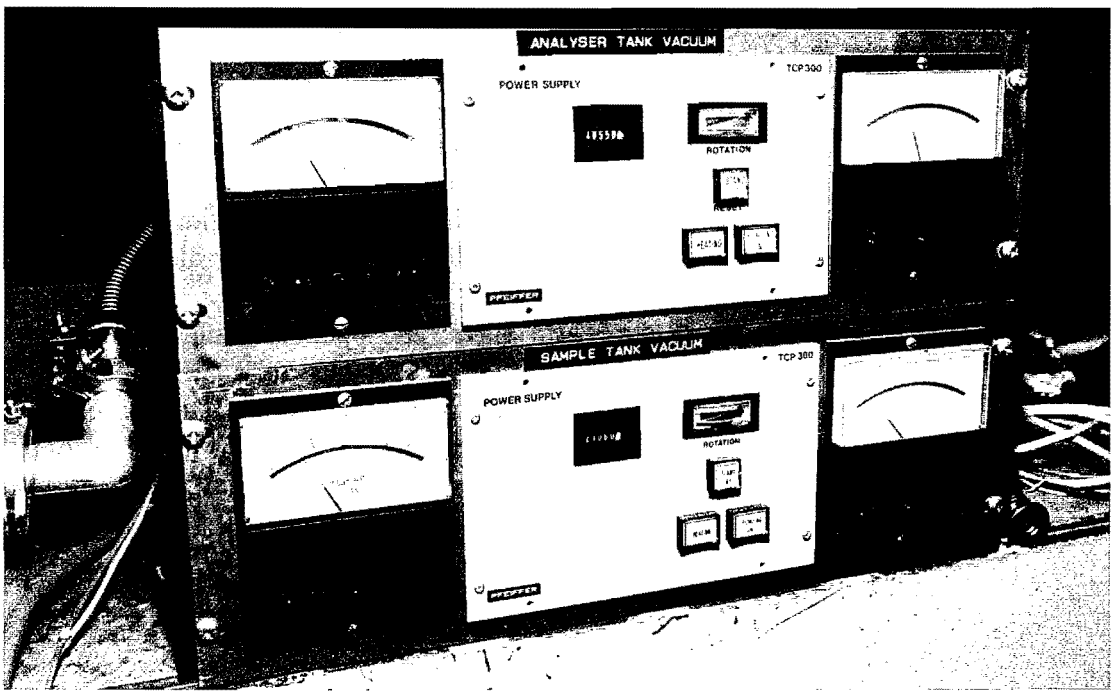


Figure 3.1.1: The vacuum gauges on TFXA *95RC1020*

Good things to look for:

1. Both units showing "PUMPING UNIT" and "HEATING" buttons illuminated.
2. Both units showing the "ROTATION" indicator on green, at extreme right.
3. Typical pressures; "ANALYSER" ~ 10^{-4} mbar, "SAMPLE" ~ 10^{-6} mbar.

3.2 Sample Environment Equipment

This section discusses the operation of the more commonly used pieces of sample environment equipment on TFXA.

3.2.1 The Top Loading CCR

The top loading CCR is the most commonly used piece of sample environment equipment used on TFXA. The cryostat attains a base temperature in the 20 - 30K range and normally requires no attention from the user. The compressor is located against the wall opposite the door to the TFXA cabin and normally shows a green light. In the unlikely event that the compressor cuts-out the light shows red. Check that the helium pressure is around 20bar, too high (>25bar) or too low (<15bar) requires adjustment. *Do not attempt this without first obtaining instructions from your local contact or a Sample Environment Technician.* If the pressure is correct then the compressor may be re-started.

3.2.2 The Orange Cryostat

The use of the orange cryostat is described in RAL reports 93-006 and 92-041, copies of which are kept in the TFXA cabin. The table below provides brief information concerning valve settings and flow rates. Both the warm and cold valves should only be finger tight. Over tightening them will cause damage.

Cooling to >4K	Open the cold valve 1/2 turn. Open the warm valve until the flow observed on the gas recovery flow meter is 10L/min
Constant temperature >4K	Once the required temperature has been reached reduce the flow to 5L/min using the warm valve, and the temperature will be controlled by the Eurotherm and the cryostat heater, or, if you want the temperature to remain stable at 4K, switch the heater off.
Cooling to <4K	Close the warm valve, and open the cold valve 1/2 turn. Slowly open the Rootes pump valve, never letting the pressure rise to above 10 torr. When the pump valve is fully open control the flow to about 0.5 to 1Litre/min by adjusting the cold valve. This is non trivial.

3.3 Electronics

The electronics rack contains the hardware for the detectors and is located by the pillar crane on top of the mezzanine.

You will **NOT** normally touch any of this equipment, however you should check all is working.

Good things to look for:

1. Be filter temperatures showing less than 100K (located at the top of the rack).

2. "Le Croy" HT supplies showing 850 volts (located at the bottom of the rack).

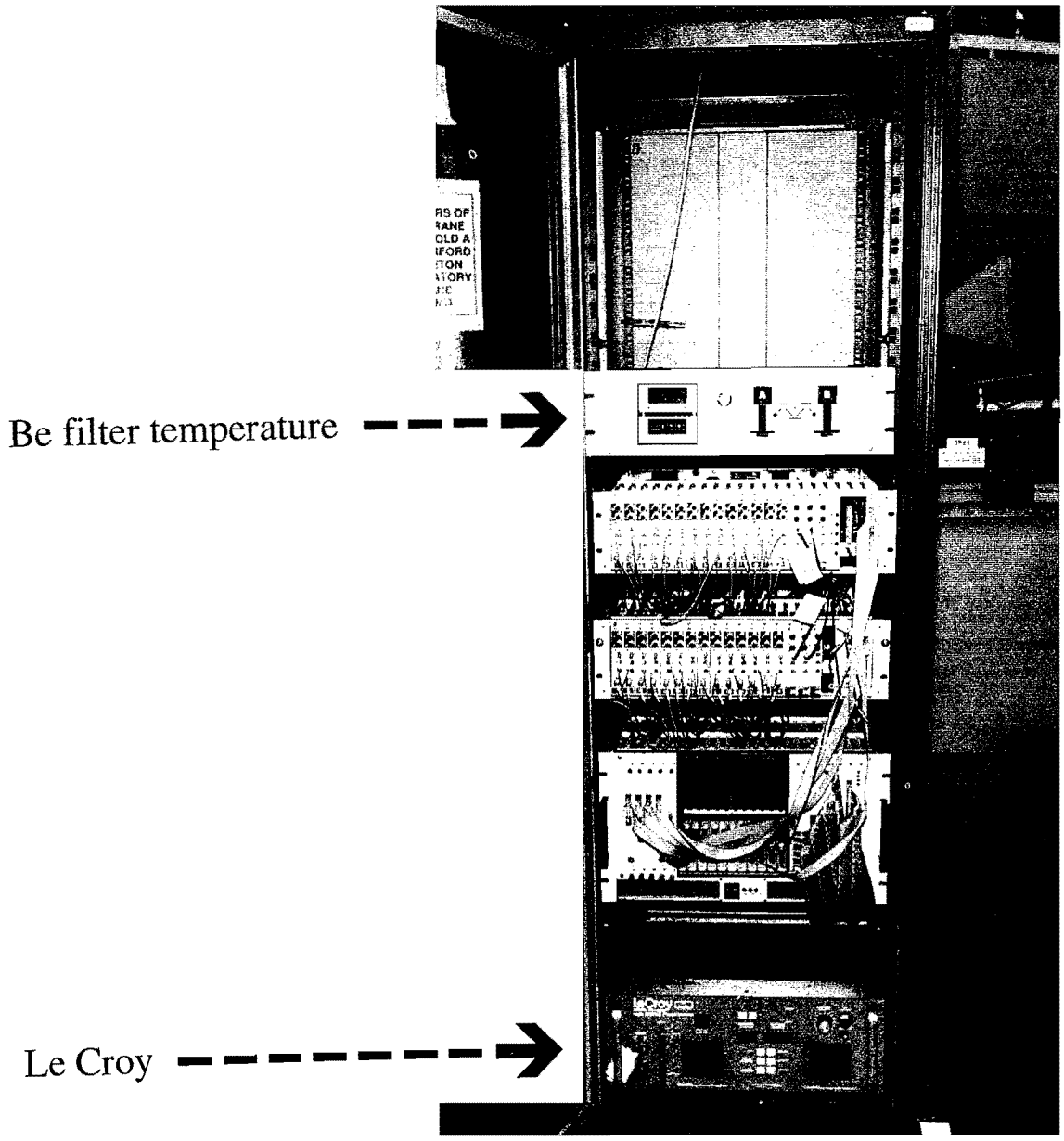


Figure 3.4.1: Photograph of electronics rack. *95RC3072*

4. CONTROLLING THE INSTRUMENT

The terminal in the cabin usually has four windows, as shown in *Figure 4.1*. The Dashboard provides a display of all the instrument parameters, including the sample and CCR temperature. There is a TFXA 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 `tfxa$disk0:[tfxa.work]` area at all times. There will also be a GENIE window and the GKS graphics window that goes with it. There may also be a horizontal strip labelled "Session Manager".

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

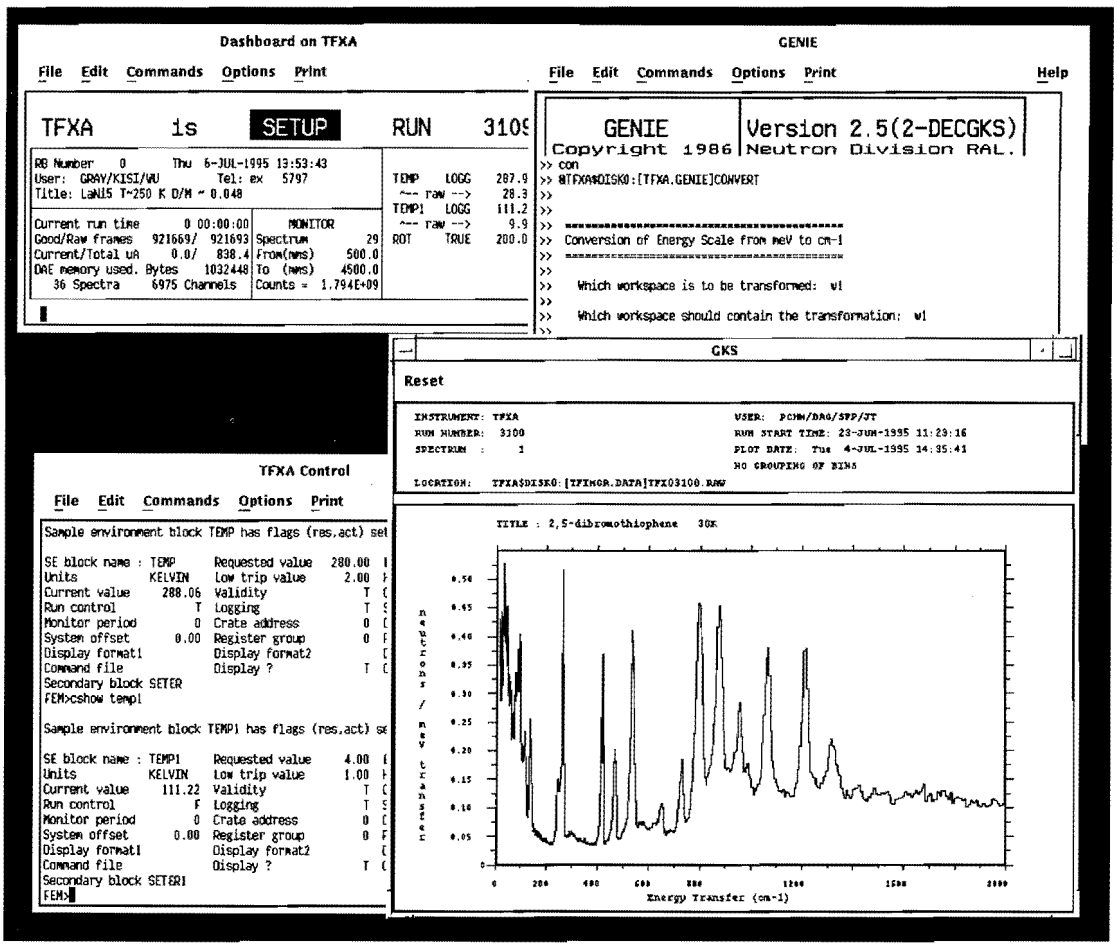


Figure 4.1: Typical display on the terminal in the TFXA cabin.

(Note: Where given ↵ requires a carriage return, where it is not given it is implied, except if [brackets] are used).

4.1 Change

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

`FEM> 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 TFXA form a unique library whose usefulness is compromised if the spectra are not clearly identified.

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

4.2 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). 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 TFXA enclosure, 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. (If the orange cryostat is used then the lead goes into the "HTR" socket on the side of cryostat, in the bank marked "CENTRESTICK"). The heater on/off switch is on the Eurotherm crate, in the electronics rack in the TFXA cabin. On the back of the Eurotherm crate there is a rotary switch to set the heater voltage (Maximum voltage = 36V).

4.3 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 `tfxa$disk0:[tfxmgr.data]tfx0<xxxx>.sav`. The store command should always be preceded by an update
`pause`	Pauses data collection.
`resume`	Resumes data collection.
`abort`	Aborts the current run without saving any data.
`end`	Ends the current run and stores the data in `tfxa$disk0:[tfxmgr.data]tfx0<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.

4.4 Using Command Files

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

```
$ begin                                  begins run
$ waitfor 1000 uamps                     wait for 700µ Amps
$ 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 TFXA 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:min:secs` format used by the VMS operating system.

`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 (see the sample command file above).

5. DATA ANALYSIS AND VISUALISATION.

Several programs and utilities exist to help you analyse your data including the GAUS least squares fitting program. TFXA 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 TFXA GENIEINIT.COM. Please do not log onto TFXA and start Genie as this seriously slows the system; use a different computer instead *e.g.* ISISE.

5.1 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 TFXA cabin. Additional copies may be obtained from the computer support office.

If you are at an X terminal, the GENIE window should already be opened. At the X windows terminal in the TFXA cabin, if there is no Genie window or if Genie crashes (rare but not unknown!) it is restarted by clicking on the word TFXA on the Session Manager and then on Genie on the drop-down menu. (The Session Manager may be shrunk to an icon, in which case it can be restored by double-clicking on the icon. It may be necessary to move some of the other windows in order to find the icon, although it is usually to be found in the bottom right-hand corner of the screen).

If however, you are on a single screen terminal you will need to type :

```
FEM>genie↵
```

If using a single screen terminal, a page will then scroll past which includes each specialised function available and the command needed to utilise them. For reference a copy of which can be found in section 7.2. If you are on an X windows machine the message will not appear, just click on the GENIE window.

Note that if you are using a Falco terminal, to toggle between graphics and text, hold down the CTRL key and then press the F6 key.

On TFXA, Genie is divided into 10 workspaces, w1 - w10. The data in Genie is completely volatile and does not alter the original data on the TFXA disk.

5.1.1 Looking at analysed files

To read in an analysed file type :

```
>>r w1 [tfxa.user]trsl××××.ana↵
```

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

```
>>d w1↵
```

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

```
>>d w1 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.

5.1.2 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.

5.1.3 Overlaying spectra

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

`>>p wx↵`

Where **x** 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↵`

5.1.4 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` (see Genie manual) 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.

5.1.5 Hard copies

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

```
>>k/h↵
```

This carries out a screen dump of the Genie display window and creates a postscript file, 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 5.1.5). 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.

laser printers	**location**
LASER 0	Computer support office, R3.
LASER 1	Coffee room, R3.
LASER 2	DAC, R55.
LASER 4	CRISP portacabin
LASER11	HET portacabin

Table 5.1.5: A list of the normally used printer devices.

5.1.6 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 (or the cursor keys on a single screen terminal). When in the correct place click the left button (or return), a prompt will then appear. Type :

`:x↵` *To get the x value for the current point*

`:y↵` *To get the y value for the current point*

`:p↵` *To get both the x and the y value for the current point*

`:e↵` *To exit this mode*

5.1.7 Useful functions in Genie

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

B2A
This program converts a binary file (located in a workspace) into an ASCII format, which is suitable for CLIMAX input. Type :

```
>>b2a↵
```

Then follow the on screen instructions.

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.

QUICK_REHACK
This is to have a quick look at the spectra to make sure that everything looks satisfactory. All of the options have automatic defaults and so typing :

```
>>quick_rehack↵
```

will result in an analysed spectrum **that is not saved.** The output of **QUICK_REHACK** is placed in workspace w5. Note that workspaces w1 - w4 are overwritten during the analysis.

REHACK
This is the main TFXA data analysis program. This differs from the above as you have various options to choose between. For example, what energy range you wish to include in the analysis. For more details see section 7.2.1.

SMOOTH
This creates a smoothed spectrum. Type :

```
>>smooth↵
```

Then follow the on screen instructions.

STR
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 :

```
>>stretch↵
```

Then follow the on screen instructions.

TEMP_PLOT
This plots the temperature vs time for an old run. Type :

```
>>tp↵
```

TEMP_PLOT_CURRENT
This plots the temperature vs time for the current experiment. Type :

```
>>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:mn:sc
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/1 w1
```

"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.

TFXA_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 - 3Å in d-spacing and the resolution is $\Delta d/d \approx 3 \times 10^{-3}$. They may be analysed with **TFXA_DIFF** the diffraction analysis program. To run, type :

```
>>tfxa_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).

ADDRAW

This program allows you to add raw data files together, the net result is exactly the same as one spectrum that had been run for the same total number of μAh. This program is somewhat different from the others in this section in that it is run from the TFXA Control window:

```
FEM>ADDRAW↵
```

You are asked for the run numbers and then whether you wish to exclude any tubes. Almost always the answer is no. To analyse the new file, it is necessary to use REHACK, however, you will need to get your local contact to place the file in the correct directory.

5.1.8 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 - 28 are the inelastic detectors, tube 29 is the monitor and tubes 30,31,33,34 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.

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 TFXA Control window:

```
FEM> ISISNEWS C↵
```

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, eg 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**. Failing that either Stewart Parker or John Tomkinson.

	RAL extension	*Home number*
Stewart Parker	5797	01235 550114
John Tomkinson	6686	01491 833869

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.

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

To use the bleeper, phone 70 and wait for a tone, then dial the current extension number plus the bleeper number and wait for a tone again before replacing the receiver.

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 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 at its surface. 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 - 13.00
Dinner	17.15 - 19.15	18.00 - 19.00

R1 coffee lounge (hot drinks/snacks)	9.00 - 11.30	(Monday-Friday)
	11.45 - 15.45	"
R22 coffee lounge	11.30 - 13.45	"

These times are correct at 12/7/95. However... things can change!

6.5.2. Pubs

Blewbury	The Red Lion	
Chilton	Rose & Crown	
West Hagbourne	The Horse and Harrow	(Peter's Pub)
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 TFXA Parameters

Moderator:	H_2O 100K (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	28 ^{3}He proportional counters for inelastic scattering 4 ^{3}He diffraction detectors (6 mm effective thickness 250 mm effective length)

Distances

Moderator to Sample	12.13 m
Sample to detectors	~0.7 m

7.2 List of TFXA Specific Genie commands

```
> B2A:==@tfxa$disk0:[tfxmgr.utils]b2a
!     Converts binary files into ASCII
> CON:==@tfxa$disk0:[tfxa.genie]CONVERT
!     Conversion of X-scale from meV to cm-1
> DER:==@tfxa$disk0:[tfxa.genie]DERIVATIVE
!     Double derivative of a workspace
> GAUS:==@tfxa$disk0:[tfxa.genie]GAUS
!     Gaussian fits prog (R.Osborne)
> QUICK_REHACK:==@tfxa$disk0:[tfxa.user]rehack_quick_look_1992
!     Quick look at data to see if statistics are o.k.
> REHACK:==@tfxa$disk0:[tfxa.user]REHACKDATA
!     "Fully interactive" data reduction/analysis program
> SMOOTH:==@tfxa$disk0:[tfxa.genie]smooth
!     Smoothing routines for backgrounds
> STR:==@tfxa$disk0:[tfxa.genie]STRETCH
!     Stretches/compresses the X scale by requested factor
> TFXA_DIFF :==@TFXA$DISK0:[TFXA.genie]tfxa_diff
!     Diffraction data analysis
> TP:==@TFXA$DISK0:[TFXA.GENIE]TEMP_PLOT.COM
> TPC:==@TFXA$DISK0:[TFXA.GENIE]TEMP_PLOT_CURRENT.COM
!     Temperature plotting of current or old data
> ZERO:==@tfxa$disk0:[tfxa.genie]ZERO_ERRORS
!     Sets all error values in a workspace to zero
```

7.2.1 Rehack

The use of a fixed final energy on TFXA 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 TFXA 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 `TRSL`**xxxxx**`.ANA` in the directory `TFXA$DISK0:[TFXA.USER]` a few minutes later.

However, there are rare occasions when a manual intervention is either necessary or desired. These include analysing `.RAW` files that have been co-added using ADDRAW, the need to see below 2 or above 500 meV (data exists in the range -2 - 2000 meV), when the batch file does not run or when the `.ANA` file has been corrupted and the data has to be re-analysed. Note that the `.RAW` file is unchanged by REHACK in any of its manifestations.

To run REHACK type:

```
>>rehack↵
```

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 ΔE/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 ΔE/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 $\Delta E/E$ 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 $S(Q,\omega)$
3 for both (usual choice)
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 (±10%) 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

For the curious, a complete listing of the program follows.

```
!      REDUCEDATA  TFXA DATA REDUCTION PACKAGE
!
!      J.Penfold    J.Tomkinson
!        neutron division
!
!      MODIFIED ON 22 JULY 1987
!      By S. Robertson Neutron Division
!      To restrict naming and targeting of analysed data files.
!
!      MODIFIED on 24th April 1991
!      by A Chappell ISIS Science division
!      Parameters of detectors 18-32 adjusted
!      following movement and re-calibration of analyser
!
!
!      18 April 1992
!      A V Belushkin
!      Primary flight path changed for 12.13 m and parameters for
!      all detectors updated after realignment of analyser crystals
!
!      8 October 1993
!      A V Belushkin
!      New position for the monitor after the installation of the
!      diffraction detectors. Monitor spectrum is now s29. Detectors
!      15-18 are excluded from the analysis. From now on the INS
!      detectors are spectra 1-28 and diffraction detectors
!      are spectra 30-35.
!
!
!      7th July 1995
!      S F Parker
!      Program modified to include all detectors ie 1-28.
!      Also changed to make exclusion of detectors an option
!      (Previous version now called REHACKDATA_JUL1995.COM;24).
!
!
!
!
#########################################################################
#
!
!            initial setup
!
>set wor 16 8000
>!set inst tfx
>!set disk tfxa$disk0:
>!set dir TFXMGR.DATA
!
! ********* What is the data file extension? *********
!
$inquire Z "Enter 1 for RAW, 2 for SAV or 3 for SUM"
!
$GOTO (LZ1,LZ2,LZ3) Z
$LZ1:
>set ext .RAW
$GOTO LZ4
$LZ2:
>SET EXT .SAV
$GOTO LZ4
$LZ3:
>SET EXT .SUM
$LZ4:
!
$inquire irun "enter run no"
!
!
! energy binning options
! ibin=1  constant delta e/e
!      =2  constant delta e
$INQUIRE IBIN "ENTER BINNING OPTION"
$GOTO (LB21,LB22) IBIN
$LB22:
```

```
$INQUIRE EBIN "ENTER DELTA E BIN"
$GOTO LB23
$LB21:
!
! Note a recommended value for bin is given by : BIN=2E-4(SQRT(Emax))
! Where Emax=upper energy limit of analysis
!
$INQUIRE EBIN "ENTER DELTA E/E BIN (input in .*** format only)"
$LB23:
!
!
$inquire emin "enter emin"
$inquire emax "enter emax"
!
!   output files selection
!     1=double diff
!     2=s(q,w)
!     3=both
!     4=none
$ INQUIRE L1 "enter selected option"
!
$ INQUIRE I2 "Do you want to exclude any detectors? 1=Yes, 2=No"
$ GOTO (I10,I11) I2
$I10:
!
! setup flag array to exclude specific noisy detectors
!     1=include   0=exclude
$ DO JJ=1,28
$ IFLG=0
$ INQUIRE IFLG "enter flag for tube No.'JJ'"
$ IFLAG'JJ'=IFLG+1
$END DO
$ GOTO I12
!
$I11:
$ DO JJ=1,28
$ IFLG=2
$ IFLAG'JJ'=IFLG
$END DO
$I12:
!
>ass 'irun'
!
!            SETUP NORMALISATION
>w1=s1
>w2=s29
>set par 2 11.04 0.0 90.0 0 0.0
>u/lam w2
>fun w2 source:wexm w2
>set par 1 12.13 0.7507 90.0 2 4.8907
>u/la1 w1
>rebin w1 w2
>w4=w1/w2
>set par 4 12.13 0.7507 90.0 2 4.8907
>set ycode w4 -1
>u/w w4
$GOTO (LB31,LB32) IBIN
$LB31:
>REBIN 'EMIN' ['EBIN'] 'EMAX' W4
$GOTO LB33
$LB32:
>REBIN 'EMIN' ('EBIN') 'EMAX' W4
$LB33:
>fun w4 source:clear w4
$ DET1:
!-----------------------------------------
!           Detector 1
!-----------------------------------------
!
$GOTO (D12,D11) IFLAG1
$D11:
>W1=S1
```

```
>SET PAR 1 12.13 0.7450 90.0 2 4.7706
>U/LA1 W1
>rebin w1 w2
>W3=W1/W2
>SET PAR 3 12.13 0.7450 90.0 2 4.7706
>SET YCODE W3 -1
>U/W W3
>@tfxa$dua0:[tfxa.genie]REBOPT EMIN EBIN EMAX IBIN
>W4=W4+W3
$D12:
$ DET2:
!-----------------------------------------
!           Detector 2
!-----------------------------------------
!
$GOTO (D22,D21) IFLAG2
$D21:
>w1=s2
>set par 1 12.13 0.7346 90.0 2 4.6635
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.7346 90.0 2 4.6635
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D22:
!
$ DET3:
!-----------------------------------------
!           Detector 3
!-----------------------------------------
!
$GOTO (D32,D31) IFLAG3
$D31:
>w1=s3
>set par 1 12.13 0.7261 90.0 2 4.5564
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.7261 90.0 2 4.5564
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D32:
!
$ DET4:
!-----------------------------------------
!           Detector 4
!-----------------------------------------
!
$GOTO (D42,D41) IFLAG4
$D41:
>w1=s4
>set par 1 12.13 0.7136 90.0 2 4.4309
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.7136 90.0 2 4.4309
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D42:
!
$ DET5:
!-----------------------------------------
!           Detector 5
!-----------------------------------------
!
```

```
$GOTO (D52,D51) IFLAG5
$D51:
>w1=s5
>set par 1 12.13 0.7025 90.0 2 4.3033
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.7025 90.0 2 4.3033
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D52:
!
$ DET6:
!-----------------------------------------
!           Detector 6
!-----------------------------------------
!
$GOTO (D62,D61) IFLAG6
$D61:
>w1=s6
>set par 1 12.13 0.6929 90.0 2 4.1826
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6929 90.0 2 4.1826
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D62:
!
$ DET7:
!-----------------------------------------
!           Detector 7
!-----------------------------------------
!
$GOTO (D72,D71) IFLAG7
$D71:
>w1=s7
>set par 1 12.13 0.6829 90.0 2 4.0591
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6829 90.0 2 4.0591
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D72:
!
$ DET8:
!-----------------------------------------
!           Detector 8
!-----------------------------------------
!
$GOTO (D82,D81) IFLAG8
$D81:
>w1=s8
>set par 1 12.13 0.6728 90.0 2 3.9446
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6728 90.0 2 3.9446
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D82:
!
!$ DET9:
```

```
!-----------------------------------------
!           Detector 9
!-----------------------------------------
!
$GOTO (D92,D91) IFLAG9
$D91:
>w1=s9
>set par 1 12.13 0.6629 90.0 2 3.8250
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6629 90.0 2 3.8250
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D92:
!
$ DET10:
!-----------------------------------------
!           Detector 10
!-----------------------------------------
!
$GOTO (D102,D101) IFLAG10
$D101:
>w1=s10
>set par 1 12.13 0.6531 90.0 2 3.7004
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6531 90.0 2 3.7004
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D102:
!
$DET11:
!-----------------------------------------
!           Detector 11
!-----------------------------------------
!
$GOTO (D112,D111) IFLAG11
$D111:
>w1=s11
>set par 1 12.13 0.6455 90.0 2 3.5964
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6455 90.0 2 3.5964
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D112:
!
$ DET12:
!-----------------------------------------
!           Detector 12
!-----------------------------------------
!
$GOTO (D122,D121) IFLAG12
$D121:
>w1=s12
>set par 1 12.13 0.6327 90.0 2 3.4876
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6327 90.0 2 3.4876
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
```

```
>w4=w4+w3
$D122:
!
$ DET13:
!-----------------------------------------
!           Detector 13
!-----------------------------------------
!
$GOTO (D132,D131) IFLAG13
$D131:
>w1=s13
>set par 1 12.13 0.6252 90.0 2 3.3848
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6252 90.0 2 3.3848
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D132:
$ DET14:
!-----------------------------------------
!               Detector 14
!-----------------------------------------
!
$GOTO (D142,D141) IFLAG14
$D141:
>w1=s14
>set par 1 12.13 0.6176 90.0 2 3.2786
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6176 90.0 2 3.2786
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D142:
$ DET15:
!-----------------------------------------
!           detector 15
!-----------------------------------------
!
$GOTO (D152,D151)IFLAG15
$D151:
>w1=s15
>set par 1 12.13 0.6215 90.0 2 3.2014
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6215 90.0 2 3.2014
>set ycode w3 -1
>u/w w3
>@source:rebopt emin ebin emax ibin
>w4=w4+w3
$D152:
$ DET16:
!-----------------------------------------
!           detector 16
!-----------------------------------------
!
$GOTO (D162,D161)IFLAG16
$D161:
>w1=s16
>set par 1 12.13 0.6070 90.0 2 3.1616
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6070 90.0 2 3.1616
>set ycode w3 -1
>u/w w3
```

```
>@source:rebopt emin ebin emax ibin
>w4=w4+w3
$D162:
$ DET17:
!
!
!-------------------------------------------
!           DETECTOR 17
!-------------------------------------------
!
$GOTO (D172,D171) IFLAG17
$D171:
>W1=S17
>SET PAR 1 12.13 0.5904 90.0 2 2.9942
>U/LA1 W1
>rebin w1 w2
>W3=W1/W2
>SET PAR 3 12.13 0.5904 90.0 2 2.9942
>SET YCODE W3 -1
>U/W W3
>@source:REBOPT EMIN EBIN EMAX IBIN
>W4=W4+W3
$D172:
$ DET18:
!
!
!-------------------------------------------
!           detector 18
!-------------------------------------------
!
$GOTO (D182,D181) IFLAG18
$D181:
w1=s18
>set par 1 12.13 0.6193 90.0 2 3.2218
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6193 90.0 2 3.2218
>set ycode w3 -1
>u/w w3
>@source:rebopt emin ebin emax ibin
>w4=w4+w3
$D182:
$ DET19:
!-------------------------------------------
!           Detector 19
!-------------------------------------------
!
$GOTO (D192,D191) IFLAG19
$D191:
>w1=s19
>set par 1 12.13 0.6209 90.0 2 3.2864
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6209 90.0 2 3.2864
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D192:
!
$ DET20:
!-------------------------------------------
!           Detector 20
!-------------------------------------------
!
$GOTO (D202,D201) IFLAG20
$D201:
>w1=s20
>set par 1 12.13 0.6327 90.0 2 3.3935
>u/la1 w1
```

```
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6327 90.0 2 3.3935
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D202:
!
$ DET21:
!-----------------------------------------
!           Detector 21
!-----------------------------------------
!
$GOTO (D212,D211) IFLAG21
$D211:
>w1=s21
>set par 1 12.13 0.6418 90.0 2 3.4992
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6418 90.0 2 3.4992
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D212:
!
$ DET22:
!-----------------------------------------
!           Detector 22
!-----------------------------------------
!
$GOTO (D222,D221) IFLAG22
$D221:
>w1=s22
>set par 1 12.13 0.6484 90.0 2 3.5999
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6484 90.0 2 3.5999
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D222:
!
$ DET23:
!-----------------------------------------
!           Detector 23
!-----------------------------------------
!
$GOTO (D232,D231) IFLAG23
$D231:
>w1=s23
>set par 1 12.13 0.6585 90.0 2 3.7035
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6585 90.0 2 3.7035
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D232:
!
$ DET24:
!-----------------------------------------
!           Detector 24
!-----------------------------------------
!
$GOTO (D242,D241) IFLAG24
```

```
$D241:
>w1=s24
>set par 1 12.13 0.6683 90.0 2 3.8201
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6683 90.0 2 3.8201
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D242:
!
$ DET25:
!-----------------------------------------
!           Detector 25
!-----------------------------------------
!
$GOTO (D252,D251) IFLAG25
$D251:
>w1=s25
>set par 1 12.13 0.6802 90.0 2 3.9406
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6802 90.0 2 3.9406
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D252:
!
$ DET26:
!-----------------------------------------
!           Detector 26
!-----------------------------------------
!
$GOTO (D262,D261) IFLAG26
$D261:
>w1=s26
>set par 1 12.13 0.6897 90.0 2 4.0573
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.6897 90.0 2 4.0573
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D262:
!
$ DET27:
!-----------------------------------------
!           Detector 27
!-----------------------------------------
!
$GOTO (D272,D271) IFLAG27
$D271:
>w1=s27
>set par 1 12.13 0.7012 90.0 2 4.1845
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.7012 90.0 2 4.1845
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D272:
!
$ DET28:
!-----------------------------------------
```

```
!           Detector 28
!-----------------------------------------
!
$GOTO (D282,D281) IFLAG28
$D281:
>w1=s28
>set par 1 12.13 0.7133 90.0 2 4.3106
>u/la1 w1
>rebin w1 w2
>w3=w1/w2
>set par 3 12.13 0.7133 90.0 2 4.3106
>set ycode w3 -1
>u/w w3
>@tfxa$dua0:[tfxa.genie]rebopt emin ebin emax ibin
>w4=w4+w3
$D282:
!
>fun w4 source:k1k2 w5
!
! Get rid of 1e-9 factor
!
>w4=w4*1e9
>w5=w5*1e9
!
!
$ GOTO (LZ5,LZ6,LZ7) Z
$ LZ5:
$ GOTO (LB11,LB12,LB13,LB14) L1
$ LB11:
>write/open w4 TFXA$DISK0:[TFXA.USER]TRDD'IRUN'.ANA
>write/close
$ GOTO LB14
$ LB12:
>write/open w5 TFXA$DISK0:[TFXA.USER]TRSL'IRUN'.ANA
>write/close
$GOTO LB14
$ LB13:
>write/open w4 TFXA$DISK0:[TFXA.USER]TRDD'IRUN'.ANA
>write/open w5 TFXA$DISK0:[TFXA.USER]TRSL'IRUN'.ANA
>write/close
$GOTO LB14
$ LZ6:
$ GOTO (LB15,LB16,LB17,LB14) L1
$ LB15:
>write/open w4 TFXA$DISK0:[TFXA.USER]TSDD'IRUN'.ANA
>write/close
$ GOTO LB14
$ LB16:
>write/open w5 TFXA$DISK0:[TFXA.USER]TSSL'IRUN'.ANA
>write/close
$GOTO LB14
$ LB17:
>write/open w4 TFXA$DISK0:[TFXA.USER]TSDD'IRUN'.ANA
>write/open w5 TFXA$DISK0:[TFXA.USER]TSSL'IRUN'.ANA
>write/close
$ LZ7:
$ GOTO (LB18,LB19,LB20,LB14) L1
$ LB18:
>write/open w4 TFXA$DISK0:[TFXA.USER]TSUMDD'IRUN'.ANA
>write/close
$GOTO LB14
$ LB19:
> write/open w5 TFXA$DISK0:[TFXA.USER]TSUMSL'IRUN'.ANA
> write/close
$ GOTO LB14
$ LB20:
> write/open w4 TFXA$DISK0:[TFXA.USER]TSUMDD'IRUN'.ANA
> write/open w5 TFXA$DISK0:[TFXA.USER]TSUMSL'IRUN'.ANA
> write/close
$LB14:
!
*****************************************************************
```

```
!     w4 contains counts proportional to double diff cross-section
!     w5 contains counts proportional to s(q,w)
!
!     FILENAME CODE     T=TFXA
!                 R=RAW, S=SAV, SUM=SUM
!                 SL=S(Q,w),DD=DOUBLE DIFF
!
*********************************************************************
!      THE CONTROL IS NOW RETURNED TO THE KEYBOARD
```

7.3 Detector Tables

7.3.1 WIRING.DAT

Number of detectors Number of monitors
36 2

Index	Detector	Time reg	Crate	Module	Position	Monitor	M.prescale
1	1	1	0	0	0	0	0
2	2	1	0	0	1	0	0
3	3	1	0	0	2	0	0
4	4	1	0	0	3	0	0
5	5	1	0	0	4	0	0
6	6	1	0	0	5	0	0
7	7	1	0	0	6	0	0
8	8	1	0	0	7	0	0
9	9	1	0	1	0	0	0
10	10	1	0	1	1	0	0
11	11	1	0	1	2	0	0
12	12	1	0	1	3	0	0
13	13	1	0	1	4	0	0
14	14	1	0	1	5	0	0
15	15	1	0	2	0	0	0
16	16	1	0	2	1	0	0
17	17	1	0	2	2	0	0
18	18	1	0	2	3	0	0
19	19	1	0	2	4	0	0
20	20	1	0	2	5	0	0
21	21	1	0	2	6	0	0
22	22	1	0	2	7	0	0
23	23	1	0	3	0	0	0
24	24	1	0	3	1	0	0
25	25	1	0	3	2	0	0
26	26	1	0	3	3	0	0
27	27	1	0	3	4	0	0
28	28	1	0	3	5	0	0
29	29	1	0	4	0	1	2
30	30	1	0	1	6	0	0
31	31	1	0	1	7	0	0
32	32	1	0	4	1	0	0
33	33	1	0	3	6	0	0
34	34	1	0	3	7	0	0
35	35	1	0	4	2	0	0
36	36	1	0	4	3	2	2

7.3.2 SPECTRA.DAT

Number of detectors
36

Detector	Spectrum
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
16	16
17	17
18	18
19	19
20	20
21	21
22	22
23	23
24	24
25	25
26	26
27	27
28	28
29	29
30	30
31	31
32	32
33	33
34	34
35	35
36	36

7.3.3 DETECTOR.DAT

Number of detectors, Number of user table parameters/detector
36 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	4.184	.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

7.4. Detector Voltages

LeCroy Channel	Voltage	Comment
1	0	Not used
2	850	Bank 'B1'
3	850	Bank 'B2'
4	975	Monitor
5	0	Not used
6	0	Not used
7	850	Bank 'A1'
8	850	Bank 'A2'
9	850	Diffraction detector
10	850	Diffraction detector

8. INDEX

9. COMMENTS/NOTES