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The HET Mini-Manual

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The HET *mini*-manual

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1. Introduction

This document is designed to get you started planning your experiment and analysing your data. A more comprehensive user manual is being prepared. Some chapters have been completed and they can be obtained from your local contact, in addition, several RAL reports concerning the operation of sample environment equipment already exist and these can also be obtained from your local contact, although copies are kept in the instrument cabin. A PUNCH manual miniguide and Genie manual are available from the user support office.

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 arrived outside working hours. You will be issued with safety instructions which you must please read, particularly if you are a first time visitor to ISIS.
- You have picked up a film badge from the Health Physics Office opposite the MCR.
- You or your local contact have picked up the sample record sheet from the Data Analysis Centre (DAC) and that you understand the sample handling instructions.
- You thoroughly understand the operation of the safety interlock system. Your local contact will explain this to you..

When you are in the Experimental Hall outside normal working hours you must sign in at the MCR, and sign out as you leave.

1.1. Contact Numbers and the Telephone System

In the event of any problems with the instrument, computing or sample environment, your first point of contact is your local contact, failing that any member of the HET team. The names and contact numbers of the HET team are

	RAL extension	Home	Bleep
Roger Eccleston	6437	0491 834505	161
Toby Perring	5428	0734 860009	
Peter Fabi	5428		

- To dial an office extension from outside RAL dial 0235 44 followed by the extension number eg. 0235 446437.
- To make an external call from a RAL phone dial 9 before the number eg. 9 0491 834505.
- To bleep somebody dial 70 followed by the bleep number followed by the extension number you are calling from. For example to bleep Roger from HET (extension 5359) dial 70 161 5359. Wait for the tone before replacing the receiver.

1.2. Computing

When you arrive your local contact can help arrange a computer account for you. To run the software described hereafter it is important that you have the HET login.com. Your local contact can help you with this. Your local contact will also be able to help you with most computing problems, particularly those relating to instrument specific software. During normal working hours, help is also available from Computer Support on extension 3029 or by sending e-mail to **support**.

2. An Introduction to HET.

Inelastic neutron scattering may be successfully performed on a pulsed source using two types of instrument: direct geometry or chopper spectrometers, or indirect geometry or crystal analyser spectrometers. HET and MARI are examples of the former, in which a single incoming energy is selected, and the final energy and momentum transfer is analysed by time-of-flight and detector angle. The later technique involves using a white beam of neutrons and determining the incident energy by time-of-flight. At the ISIS facility, IRIS, PRISMA, eVS, TFXA and ROTAX are indirect geometry instruments.

2.1. The Neutron Inelastic Scattering Experiment on a Chopper Spectrometer.

In any neutron scattering experiment, the quantity that is being measured is the partial differential cross section,

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{\begin{pmatrix}\text{number of neutrons scattered per second into a small solid angle} \\ d\Omega \text{ in the direction} \theta,\ \phi \text{ with final energy between E and E'+dE'}\end{pmatrix}}{\phi d\Omega dE'}.$$

σ is scattering cross section.

The quantity of interest is actually the scattering function or scattering law $S(\mathbf{Q},\omega)$ where

$$\frac{d^2\sigma}{d\Omega dE} = \frac{\sigma}{4\pi}\frac{\mathbf{k}_f}{\mathbf{k}_i} NS(\mathbf{Q},\omega)$$

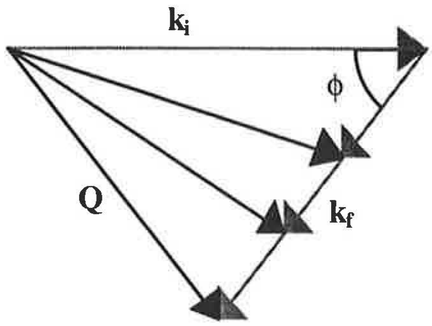
and N is the number of nuclei in the scattering system.

Thus, we measure $S(\mathbf{Q},\omega)$ as a function of energy transfer $\hbar\omega$ and momentum transfer $\mathbf{Q}$.

$$\hbar\mathbf{Q} = \hbar\mathbf{k}_i - \hbar\mathbf{k}_f \quad \lambda = \frac{h}{mv} \quad \mathbf{k} = \frac{2\pi}{\lambda} \quad \mathbf{k} = \frac{mv}{\hbar}$$

$$\hbar\omega = \frac{\hbar^2}{2m}\left(\mathbf{k}_i^2 - \mathbf{k}_f^2\right)$$

$$E = \hbar\omega \qquad E = \frac{\hbar^2\mathbf{k}^2}{2m}$$



In a neutron scattering experiment conducted on a chopper spectrometer, the neutrons arrive at the sample in monochromatic pulses of known energy. After scattering from the sample they are detected in fixed arrays of detectors as a function of their total time-of-flight. With a knowledge of the sample detector distances and the incident beam energy, the final energies can be calculated. At any one of the detectors a wide range of energies may be absorbed. For all energies, the final wavevector will lie along the same direction, however, the magnitude will decrease with the velocity of the incident neutrons. The scattering triangle is thus altered in time as shown.

By applying the cosine rule to the scattering triangle, bearing in mind that $\mathbf{k_i}$ is fixed and translating into energy units, it can be clearly seen that a detector positioned at a scattering angle ϕ will perform a scan in time whose loci is a parabola in $\mathbf{Q},\omega$ space.

The scan performed by each detector is dictated by the scattering angle of that detector and the incident energy.

$$\mathbf{Q}^2 = \mathbf{k}_i^2 + \mathbf{k}_f^2 - 2\mathbf{k}_i\mathbf{k}_f\cos\phi$$

$$\frac{\hbar^2\mathbf{Q}^2}{2m} = E_i + E_f - 2\left(E_iE_f\right)^{1/2}\cos\phi$$

$$\frac{\hbar^2\mathbf{Q}^2}{2m} = 2E_i - \hbar\omega - 2\cos\phi\left[E_i\left(E_i - \hbar\omega\right)\right]^{1/2}$$

2.2. Components of a Chopper Spectrometer.

The components of a chopper spectrometer such as HET are shown in the schematic diagram, figure 1, alongside examples of the neutron spectra at each point along the path of the neutron. The proton pulse hitting the target produces a burst of very fast, very high energy neutrons. To slow these down to usable energies the high scattering cross section of hydrogen is utilised. Hydrogen at 22K, CH_2 at 100K and H_2O at 316K are used as **moderators**. In order to preserve the high flux of high energy neutrons which is a valuable feature of pulsed sources the beam is undermoderated. That is to say the neutron flux leaving the moderator has two components; the Maxwellian component caused by the moderation and the epithermal (high energy flux) of the weakly moderated neutrons.

A substantial amount of background arises from γs generated as the proton beam hits the target and from fast neutrons which thermalise within the spectrometer. Consequently the background is reduced significantly by using a **nimonic chopper** which effectively closes the beam tube to the spectrometer at the moment the proton beam is incident on the target.

The beam itself is monochromated by a **Fermi chopper**, which is an aluminium drum with thin sheets of highly absorbing material such as boron, interleaved with neutronically transparent sheets of aluminium. The rotation of the drum is phased to the ISIS pulse and is only in transmitting position at the point at which it will only transmit neutrons with the desired velocity and hence $\mathbf{k}_i$ and E_i. In practice the slits are curved in opposition to the direction of rotation to optimise transmission. The chopper drum becomes increasingly grey as the energy increases. This greyness gives rise to a modulated background. This has been reduced by installing B_4C cheeks in the chopper bodies, but still needs to be accounted for when analysing data.

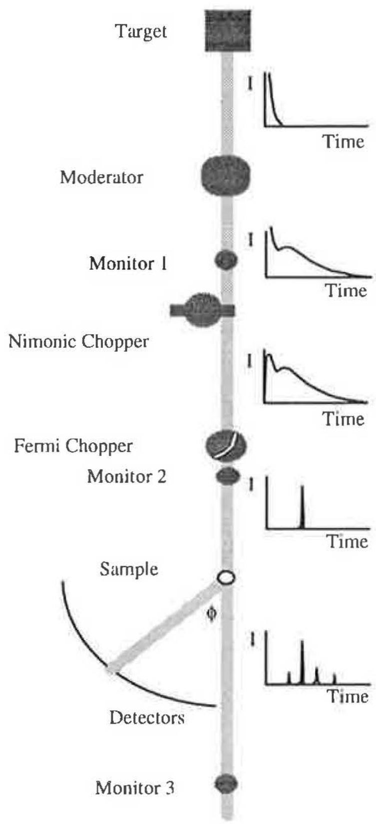


Figure 1 Schematic diagram of a chopper spectrometer.

Monitors are located at the positions indicated on the schematic diagram of the spectrometer. The time-of-flight between monitors 2 and 3 is used to determine the incident energy.

The sample is mounted on a variety of sample environment including cryostats, pressure cells and furnaces all with a standard 17" Tomkinson flange. The tank itself is evacuated to a cryogenic vacuum during an experiment. The beam tubes and detector tanks are evacuated to a rough vacuum thus reducing the background arising from air scattering.

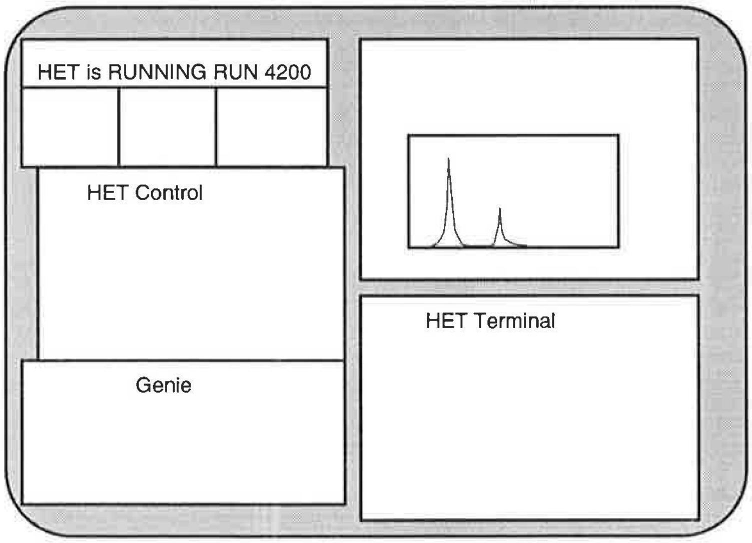
The size of the neutron beam falling on the sample is determined by the extent to which the beam has been collimated and apertures at the entry to the sample tank. The final **aperture** may be altered by changing the final collimation piece. In the near future, motorised jaws will be installed to allow tailoring of the beam dimensions to suit the sample and sample environment.

All internal surfaces in the sample tank are lined with a low hydrogen B_4C resin mix which minimises the background arising from the scattering of high energy neutrons. B_4C is also used as a shield behind the detectors.

HET is equipped solely with 10 atmosphere ^{3}He **detectors**. The specifications of HET as of February 1994 are summarised in the table in section 7.

3. Controlling the Instrument

The terminal in the cabin usually displays five windows, conventionally arranged as shown below. The dashboard at the top left hand corner of the screen provides a display of all the instrument parameters, including sample temperature goniometer angles etc. Where possible, the HET control window should only be used for control commands such as beginning, updating and ending runs, changing incident energies or temperatures, and starting instrument control command files. If this convention is adhered to it is easy to follow the status of the instrument. All data analysis should be performed in the HET terminal window. The GENIE windows are used for data display.



3.1. Selecting a Chopper Slit Package and Frequency

Four chopper slit packages are used on HET, and their specification are given in the following table.

Slit package	Optimum E_i	Comments
A	500 meV	
B	250 meV	
C	100 meV	
S	500 meV	relaxed resolution

The program **CHOP**, written by Toby Perring, calculates the flux and resolution expected for a given chopper running at a given frequency. It has been well documented elsewhere and will only be briefly described here. To run the program use the HET Terminal window, and type **CHOP**. You will then be prompted to give the instrument name. The chopper frequency is often given in terms of multiples of the ISIS pulse (50Hz). At the arrow prompt you select a chopper and frequency using the command

> **s c** <frequency/isis> <slit package>

For example, **s c 10b** selects the B chopper spinning at 500Hz. To plot out the flux and resolution use the command

> **p c** <E_i min> <E_i max>

Another chopper can now be selected using the **s c** command and plotted on the same axis using the command

> **p o c**

To obtain values for the resolution and flux for a particular slit package and frequency at a specific incident energy, select the slit package and frequency as before, then set the incident energy using the command

>**set ei** <Ei>

The flux and resolution can then be displayed using the commands

>**d f**

and

>**d r**

respectively. The command to leave chop is **ex**.

3.2. Setting the Incident Energy

To set the incident energy use the command

HET>**set_ei** <Ei(meV)> <frequency(Hz)> <slit package>

This command will set the necessary phase and frequency, and also write the file, TCB.DAT, which will be loaded into the instrument control program (ICP) the next time a change or load command is issued. *For this reason, it is crucial that a change command is issued after the energy is set. It is also vital that the* **set_ei** *command is issued from the* het$disk0:[het.run] *area and that the* **change** *or* **load** *command is issued from the same area.* The LED display on the chopper control crate in the instrument cabin displays the chopper frequency and the small LED to the left will be alight until the chopper has phased correctly. Wait until the correct chopper frequency has been established and the phase is correct before starting a run. If the phase LED is still alight more than 30 seconds after the desired frequency has been established, move the small switch below the frequency display from **comp**. to **man**., press the enter data button and return the switch to the comp. position. If the light is still on inform your local contact.

Once a run has started, it is possible to check that the chopper has phased correctly to give the desired incident energy using the following commands in the Control window.

HET>**update**
HET>**ei crpt**

The **ei** command calculates E_i from the arrival of the elastic line at monitor three, it can also be used to find the incident energy of an earlier run by simply giving the run number rather than typing CRPT.

3.3. Change

The change command allows the user to edit the dashboard information and to modify the ICP parameters.

Typing the command

HET>**change** (can be abbreviated to **cha**)

will initiate the dashboard editor. Move between areas using the cursor keys and over type or toggle, using the . key on the keypad, as instructed. The first page contains title and user information. When entering the title please follow the convention

<sample> <temperature> <sample environment> <Ei> <frequency/isis> <slit package>

eg $YBa_2Cu_3O_7$ T=14K CCR 100meV 10c

The rest of the editor is straightforward. Do not alter the spectra, detector or wiring tables. Unless you are making a white beam measurement ensure that the bar half way down the last page is toggled so that the TCB.DAT file is read rather than using the time channel information given below it.

To exit press **[PF1(GOLD)] e.**

If you intend to set a command file running to change energy or temperature automatically the ICP parameters can be written to a file using the **nextrun** <filename> command and loaded into the ICP using the **load** <filename> command.

HET> **nextrun** <filename>

will have the same effect as issuing a change command, but when you exit, the parameters will be written to <filename>.dat. Again, it is important to make sure that this command is issued from het$disk0:[het.run]. Examples of running the instrument using command files are given later.

3.4. Setting Sample Environment Parameters

The top right hand portion of the dashboard displays sample environment parameters such as head temperature, sample temperature and goniometer angles. To change any of these parameters the set command is used as follows.

HET>**cset t_head 10**	*will set the head requested value to 10K*
HET>**cset wccr 45**	*will move the omega table to 45°*

The temperature is usually controlled using the head sensor, although limits can be set to ensure that data are only collected between specified limits.

HET>**cset t_samp/control/lolimit=40/hilimit=50 45**

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. Unless you are using the furnace, the temperature will be controlled using the head sensor.

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

HET>**cset t_samp/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 t_head** command, check that the heater is switched on. The switch is on the right hand side of the Eurotherm crate, in the left hand rack in the cabin. On the back of the Eurotherm crate there is a rotary switch to set the heater power. Use the tables below for reference. The max_power is set in the same way as the temperature, eg.

HET> **cset max_power 50**

	Maximum Temperature	10K	30K	50K	150K	300K
orange cryostat	Heater Voltage	24V	46V	52V	60V	72V
	max_power	50	50	50	50	100
ccr	Heater Voltage	12V	24V	32V	60V	72V
	max_power	50	100	100	100	100

The variation of the head and sample temperatures over time can be studied by plotting the temperature logs using GENIE. The following set of commands in GENIE will load the sample, then the head log files and plot both on the same axes.

```
>>@g:t_cur
>>d/l w1
>>@g:t_head_cur
>>p/l w1
```

3.5. Data Collection Commands

All the following instrument control commands may be abbreviated to three letters. Instrument control commands should be issued form the CONTROL window whenever possible.

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 HET$DISK0:[HETMGR.DATA]HET0<run no.>.SAV. The store command should always be preceded by an update.
pause	Pauses data collection.
resume	Resumes data collection.
abort	Aborts the current run without saving any data.
end	Ends the current run and stores the data in HET$DISK0:[HETMGR.DATA]HET0<run no.>.RAW.

A command file, UPD_UAMP, will perform an update and a store at given intervals in total beam current. This will ensure that you will not loose all your data if there are any problems with the DAE during the run. Run UPD_UAMP from the Control window using the command

HET>**@upd_uamp** <current at first update> <interval between updates in μAmphrs> <current at final update>

To stop the command file before the final value for the total current has been reached type **[Ctrl]Y**

3.6. Using Command Files

Command files can be written to control the instrument. An example command file follows

$ set def het$disk0:[het.run]	*sets the default directory*
$ on error then continue	*ensures that the command file will continue in the event of a CAMAC error*
$ waitfor 700 uamps	*waits until the total current reaches 700μ Amps*
$ end	*end the current run*
$ cset t_head 80	*sets the head temperature*
$ cset t_samp/control/lolimit=75/hilimit=85 80	*sets temperature limits*
$ wait 00:40:00	*waits 40 mins for the temperature to stabilise*
$ load ndnio_80.dat	*loads the new icp parameters which have been written to the file* ndnio_80.dat *as described in section 2.3.*
$ begin	*begins the next run*
$ waitfor 500 uamps	
$ update	
$ store	
$ waitfor 700 uamps	
$ end	
$ set_ei 100 250 c	*sets* E_i *for the next run*
$ wait 00:15:00	*waits 15 mins for the chopper to phase*
$ load ndnio_100.dat	
$ begin	
$ waitfor 700 uamps	
$ exit	*leaves the command file*

A command file can be run from the terminal using @<filename> or as a batch job on the HET slow queue. The advantage of using a batch job is that it is possible to stop, start and alter a command file remotely. The disadvantage is that it is not obvious to anybody sitting at the instrument terminal that the instrument is being controlled by a command file. Please run all command files, and start batch jobs, from the Control window to reduce the chances of confusion.

To submit a batch job use the symbol shq thus;

HET>**shq** <filename>.

Check that the file is being executed by viewing the queue

HET>**qh**

To stop a batch job use the halt command

HET> **halt** <entry no.> **het$slow**

The entry number identifies the job and is displayed with the queue information. The progress of the command file can be monitored by viewing the log file, which is written to SYS$SCRATCH. Use the type command as follows

HET>**ty sys$scratch:**<filename>**.log**.

Note: SYS$SCRATCH: *is the logical name for* SCRATCH$DISK:[<user id>] *and may be shortened to* SS:.

4. Sample Environment Equipment

The two most commonly used pieces of equipment on HET are the orange cryostat and the top loading ccr.

4.1. 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 HET 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.

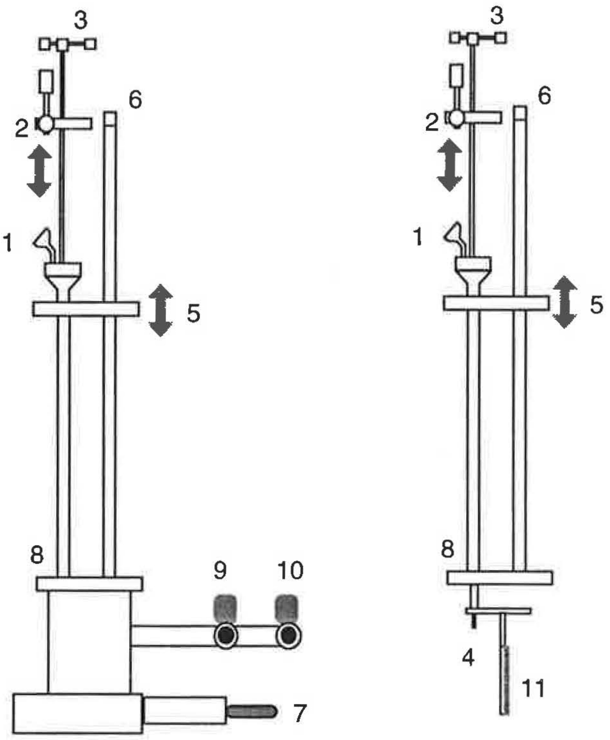
Cooling to >4K	Open the cold valve 1/2 turn. Open the warm valve until the flow observed on the gas recovery flow meter is 10L/min
Constant temperature >4K	Once the required temperature has been reached reduce the flow to approximately 4L/min using the warm valve, and the temperature will be controlled 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 use the cold valve to adjust the flow.

4.2. The Top Loading CCR

Installing the top loading ccr will have to be done by the local contact, however changing samples is very straightforward, but demands care, because there is the potential to open the sample tank to air very rapidly which will destroy the thin window between the sample and detector tanks.

4.2.1. Removing a Sample

1. Undo the sample sensor connector (1) from the top of the samplestick.
2. Undo the clamp (2) on the tightening rod (3), and lower it until it engages with the allen head bolt (4) which holds the sample holder to the cold head and unscrew it
3. Lift the sample by pulling the plate (5) all the way up the two tubes and secure it at the top with an allen screw (6).
4. Close the gate valve (7).
5. Loosen the three bolts which hold the plate onto the top of the air-lock (8).
6. Open the speed valve which lets air into the air-lock (9).
7. Undo the bolts (8) and lift the sample stick out.



4.2.1. Loading a New Sample

1. Before replacing the sample stick place a small piece of indium wire round the bolt (4) that secures the sample holder to the cold head to improve the thermal contact.
2. Replace the sample stick and finger tighten the three bolts securing it to the air-lock (8).
3. Close the air-admittance speed valve (9), and open the speed valve to the pump (10).
4. Tighten the three bolts (8).
5. WAIT for a few minutes to ensure that the air-lock has been evacuated
6. Close the speed valve to the pump (10).
7. Open the gate valve (7) SLOWLY.
8. Lower the sample (11) into position. Ensure that the plate (5) is pushed down as far as it can go.
9. Tighten the allen head bolt (4) using the tightening rod (3).
10. Withdraw the rod (3) and camp it (2) in position.
11. Replace the sample sensor connector (1).

5. Data Analysis and Visualisation.

Several programs and utilities exist to help you analyse your data including the FRILLS least squares fitting program. There is only scope here to provide the information required to allow you to produce S(ϕ,ω) plots of your data, more detailed information will be available shortly, and copies of the FRILLS manual are available. If you are doing your data analysis in your own directory make sure that you are using the HET login.com. If you are analysing data sometime after the experiment take care to explicitly state par files, using the /PAR qualifiers when running DIAG and WHITE_VAN, and mapping files, using the /MAP qualifier, when running HOMER. The default files are modified whenever the detector arrangement is altered. Make sure you make a note of the names of the mapping and par files that were in use when your data was collected.

The program HEAD is very useful if you want to find out the title, running time and total current of a previous run. It has the format

HET>**head** <run no.>

Figure 3 is a schematic layout of the HET detectors. Each detector is assigned a particular spectrum number. In most cases spectra are summed into workspaces. The rings drawn on figure 1 represent the default workspaces numbered 1 to 7 and the average ϕ angle for each workspace is given.

5.1. HOMER

The data analysis program for HET data is HOMER, which performs the following functions.

- It reads in raw data stored either in disk files (RAW or SAV files) or in the FEM memory (CRPT).
- The incident energy is automatically determined from the measured monitor spectra.
- The data are grouped into workspaces defined by a mapping file.
- Noisy or unstable detectors can be eliminated from workspaces using a mask file. This feature also allows the elimination of detectors picking up Bragg or spurious scattering
- A time-modulated or time-independent background, determined from the end of the time frame, is subtracted from the workspaces.
- The data is converted to S(ϕ,ω) i.e. converted to energy transfer and corrected for k_f/k_i and detector efficiency.
- HOMER results are usually stored in a binary file in the GENIE intermediate file format, to allow subsequent analysis within GENIE. If preferred, the workspace information can be written to an ASCII file

- An ASCII diagnostics file containing details of the HOMER analysis (incident energies, monitor integrals, spectrum integrals and backgrounds etc.) can be produced.

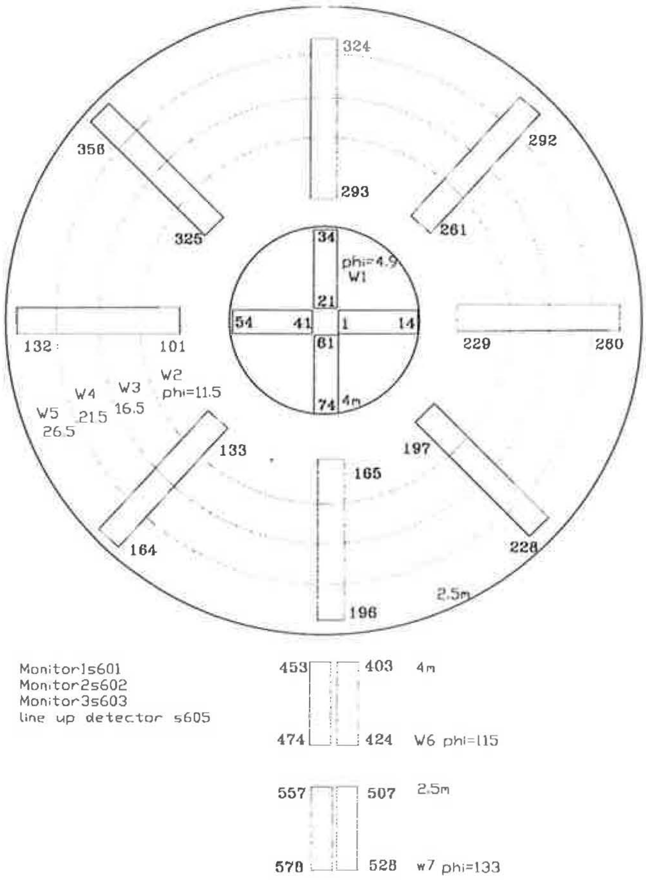


Figure 3. The HET detector layout, showing spectrum numbers, and default HOMER workspaces and their average ϕ values.

The format of the command is

HOMER <data source> (<Ei> (<Emin> (<Emax> (<dE>))))

As with all DCL commands, the user may give the shortest unambiguous abbreviation which is usually HO. The user may modify the options used by HOMER by including qualifiers in the command line. e.g.

HO/MAP=MAP:ARMS_911/MASK/VAN=2414/CHOP=400 2420

The most commonly used are described below. Other qualifiers are normally only required in exceptional circumstances.

/MAP=<map file name>

Specifies the spectrum mapping file with default extension MAP. If not given, a default ring mapping file is used (currently MAP:RINGS_934.MAP).

Note *MAP: is the logical name for* HET$DISK:[HETMGR.MAPS]. *It contains a number of commonly used mapping files. The file* AAA.TXT *contains a description of the mapping files in MAP:*

/MASK=<mask file name>

Specifies a spectrum masking file. Mask files are discussed later

/VAN=<vanadium sum file>

Specifies a white-beam vanadium sum file containing integrals from 20 to 40 meV for each detector, normalised to a default M1 sum. The integrals are used to normalise for the solid angle and detector efficiency prefactor for each detector. The sum file is either specified in full or just given as a run number, in which case the default file name is HET_DATA:HET0<run no.>.SUM or SYS$SCRATCH:HET0<run no.>.SUM.

Note HET_DATA: *is the logical name for* HET$DISK0:[HETMGR.DATA] *or* HET$DISK:[HETMGR.DATA].

/CHOP(PER_SPEED)=<chopper speed>

Specifies the speed of the chopper in Hz. This is required for the subtraction of a time modulated background.

/NORM(ALIZATION)

Determines if the data are to be normalised to the integrated monitor counts or proton current.

/OUT=<diagnostic output file name>

Specifies the name of the ASCII file containing diagnostic output. The default file specification is SYS$SCRATCH:HET0<run no.>.OUT.

/ASCII

The workspace data is written to an ASCII file, SYS$SCRATCH:HET0<run no.>.DAT.

5.1.1. Vanadium Normalisation

The white beam vanadium sum files, required by HOMER for normalisation and by the diagnostic program to create a mask file are created by the program WHITE_VAN. The command has the format.

White_van(/par=(<par file no.>) <vanadium run number>

This will create a file SYS$SCRATCH:HET0<run no.>.SUM. A copy of this file will usually have been copied by the instrument scientist to HET$DISK:[HETMGR.DATA].

5.1.2. Absolute normalisation

Scattering intensities can be put on an absolute scale in mbmeVsr^{-1} using the /ABS qualifier and calculating a constant for the normalisation from the data collected for a monochromatic vanadium run

The monochromatic vanadium data should be summed over the elastic peak using SUM as follows

SUM(/PAR=<par file no.>)**/CHOP=**<chopper frequency (Hz)>**/VAN=**<w.b. run no.>**/NORM/COR** <monochromatic van. run no.> <-xlimit> <+xlimit>

The x limits are in meV energy transfer and should be set to include all the elastic scattering from the vanadium. These values are estimated by inspecting the monochromatic vanadium data after it has been HOMERed. The qualifiers have the same meaning as they have for HOMER, except for /COR which stipulates that the data should be corrected for detector efficiency.

The summed data can now be used to derive the constant for normalisation, including the mass of the vanadium, the mass of the sample and the atomic mass of the sample. This is done using the MONO_VAN program as follows.
MONO_VAN/MV=<mass of the vanadium sample (20.14g)>**/MS=**<mass of the sample>**/AS=**<atomic mass of the sample> <monochromatic van. run no.>

The number calculated in this fashion is given the variable name MONO_COR and needs to be trimmed before being used in the HOMER command. This is done by the command

MONO_COR=F$EDIT(MONO_COR,"TRIM")

Absolute values for the scattering will now be produced if the qualifier /ABS='MONO_COR' is used in the HOMER command.

This process is made considerably easier if you use a command file to perform all the steps of the analysis. An example is given in section 4.2.

5.1.3. Mapping files

HOMER groups the recorded spectra into workspaces according to a mapping file, which is either specified by the /MAP qualifier or defined by the default value set in the current HOMER command table.

The mapping file is an ASCII file containing the following lines in free format:

1st Line:	Nw	*Nw = No. of workspaces in map*
2nd Line:	Nsp, L2,Δt,ϕ	*Nsp = No. of spectra in first workspace*
		L2 = Length of scattered flight path of first workspace (in m)
		Δ *t = Electronic time delay of detectors in first workspace (in ms)*
		ϕ *= Average scattering angle of first workspace (in °)*

3rd Line: List of spectrum nos. in first workspace (N.B. 3-9 is read as 3,4,5,6,7,8,9)
4th line: Continuation of spectrum no. list if necessary
:
The pattern, from the second line onwards, is repeated for all Nw workspaces.

The default mapping file is currently HET$DISK:[HETMGR.MAPS]RINGS_943.MAP which defines the following workspaces:

W1	4.9°	4m low angle bank
W2	11.5°	2.5m low angle bank
W3	16.5°	2.5m low angle bank
W4	21.5°	2.5m low angle bank
W5	26.5°	2.5m low angle bank
W6	115.0°	4m high angle bank
W7	133.0°	2.5m high angle bank

5.1.4. Masking Files

Masking files are used to eliminate small numbers of detectors from workspaces without the need to define a new mapping file. Common reasons for masking a detector are that

- its efficiency has varied between white beam vanadium counts
- it is relatively noisy
- it contains a Bragg peak or spurious scattering contaminating the inelastic signal.

The masking file simply consists of a list of masked spectra in free format occupying any number of lines. If the /MASK qualifier is used with the HOMER command then the default masking file (SYS$SCRATCH:HET0<run no.>.MSK) is used.

The easiest way to generate a mask file is to use the program DIAG. The format of the command is

diag/v1=<vanadium run no.>**(/v2=**<2nd vanadium run number>)(**/nozero**)(**/stab=**< stability>)(**/factor =**<factor>)**/out(/par=**<par file no.>) <run no./crpt>

DIAG will compare the two vanadium sum files and identify those detectors whose efficiency has varied between the runs and add the spectrum numbers of those detectors to the mask file, providing the /OUT qualifier is used. If the /OUT qualifier is not used, the file will not be written. It will compare the stability of detectors within a vanadium sum file and include those detectors which produce a low or high signal relative to a norm in the mask file. The data will then be searched for detectors with a high background and these will also be excluded. If the /NOZERO qualifier is not used those spectra that contain no counts will also be excluded. It is advisable to use the /NOZERO qualifier until the data has been counted for long enough to provide reasonable statistics.

5.1.5. HOMER output

The workspaces are stored in a binary file in the format required by the GENIE READ command. The default file name for this file is SYS$SCRATCH:<inst><run no>.COR. The name of this file may be changed by the /COR qualifier. A record of the HOMER analysis is stored in an ASCII file with the default file name SYS$SCRATCH:<inst><run no>.OUT if the /OUT qualifier is used. In both cases, the files may be directed to a different directory but with the same file names using the /DIR qualifier.

Note *Files stored on* SCRATCH$DISK: *will be deleted after one week, so if longer storage is required, you must use the* /DIR *qualifier, which will allow you to stipulate a destination directory, or rename the files after running HOMER.*

5.2. Command Files for Data Analysis

If you use a command file to analyse your data and keep it you have a record of the parameters and files used in your analysis. Also, re-analysis of your data is straightforward and you do not have to fill you quota with .COR files. A typical analysis command file is shown below.

```
$! This is the command file to produce .cor files for the 100meV data
$! for the NdNiO3 expt January 1994.
$!
$ sum/par=932/van=4293/chop=500/norm/cor 4309 -50 50
$ mono_van/mv=20.14/ms=36.5/as=250.95 4309
$ mono_cor=f$edit(mono_cor,"trim")
$!
$ diag/v1=het_data:het04293.sum-
      /v1=het_data:het04310.sum-
      /out-
      4305
$!
$ homer-
      /chop=500-
      /van=het_data:het04293.sum-
      /map=map:rings_934.map-
      /mask-
      /norm-
      /abs='mono_cor'
      /norebin-
      4305
```

5.2.1. Iliad.

Iliad is a command file that will perform a "first look" analysis of your data, by running DIAG and HOMER using default values and the most commonly used qualifiers. Iliad requires the sum file from the most recent white beam vanadium data. If this file has not been created you must run WHITE_VAN as described in section 4.1.1.. If you intend to look at the current run **update** the CRPT (section 2.5). In the instrument control (HET$DISK0:[HET.RUN]) area simply type

HET>**@iliad**.

You will be prompted for the run number of the data you wish to look at or type CRPT if you want to look at the current run, the chopper frequency and the number of the white beam vanadium run.

The data will be written to a .COR file as described by the default mapping file.

5.3. GENIE

GENIE is the ISIS graphics software. A full manual is included in the PUNCH user manual in the cabin and copies are available in the computer support office. Here we will briefly describe the commands which are essential for viewing HOMER data.

To run GENIE simply type GENIE.

To load HOMER workspaces, which were created using the default mapping file, into genie use the g:read command file. This command file will read in the seven workspaces described earlier and also write an eighth workspace containing the average scattering in the whole 2.5m low angle bank. If another mapping file was used the command file g:read_work should be used.

Note *g: is the logical name for* HET$DISK:[HETMGR.GENIE].

Both command files are run in genie using the format

>>@g:read

You will then be prompted for the run number and the first workspace number

The workspaces can be displayed using the command d. The plot command, p, allows you to plot the data as markers with error bars, or to plot one workspace on top of another. For example

>>d/m w1 -10 90 0 20	*plots the intensity of workspace 1 from 0 to 20 (arbitrary units) against energy transfer from -10meV to 90meV as marks.*
>>p/e w1	*adds error bars*
>>p/h w2	*overplots w2 as a histogram*

Note *d produces a new plot, p will overplot. The qualifiers, /l, /h, /e and /m correspond to lines, histograms, error bars and markers respectively.*

You may bin you data into groups using the alter bin command;

>>a b 5	*bins the data into groups of 5*

To take a hardcopy of a plot use the following two commands

>>k/h
>>j post<laser printer no.>
where the laser printer number identifies the location of the printer according to the table below.

laser printer number	**location**
0	Computer support office, R3.
1	Coffee room, R3.
2	DAC, R55.
11	HET cabin

For example, to print on the HET laser printer use

>>j post11

Once you have plotted one workspace to your satisfaction, the command file **g:precis** will automatically plot with error bars all eight workspaces and print them all on a single sheet of A4 on the HET laser printer. Precis divides workspaces 6 and 7 by five. This is an empirical figure which allows you to estimate the effects of non-magnetic background scattering on the data collected in the forward scattering banks.

6. SUMMARIES

6.1. Instrument Control

The following sequence represents the commands required to start a typical run.

HET Control

HET>tt het.run 0	*Ensure that set_ei and change are issued from het$disk0:[het.run]*
HET>**set_ei** <Ei(meV)> <freq. (Hz)> <slit package>	*eg. set_ei 100 250 c*
HET>**cset t_head** <temp>	*set the requested head temp.*
HET>**cha** Over type new title, parameters etc. **[PF1] e**	
HET>**beg**	*start the run*
HET>**upd**	*update*
HET>**ei crpt**	*Check that E_i is correct*
HET>**@upd_uamp 500 500**	*Run a command file to update and store at 500 μ Amp intervals*
. . .	
[Ctrl] y	*Stop the command file*
HET> **end**	*End the run*

6.2. Data Analysis and Visualisation

The following sequence will allow you to produce S(ϕ,ω) plots of your data, using the default settings.

HET Control

HET>**update** or **end**

HET Terminal

(HET>**White_van** <1st van run no.>
HET>**White_van** <2nd van run no.>)

HET>**diag/v1=**<1st van run no.>**/(v2=**<2nd van run no.>)**/out**(**/nozero**) <crpt or run no.>

HET>**Ho/chop=**<freq (Hz)>**/norm/van=**<van run no.>**/mask/norebin** <crpt or run no.>

(or use ILIAD)

GENIE

>>**@g:read**		*Will read in HOMER workspaces*
	run number :<run no.>	
	First workspace: **:1**	
>> **d/m w**<workspace> xmin xmax ymin ymax		*Display the given workspace*
>> **a b** <bin>		*Bin the data into groups of 'bin'*
>> **d/m**		
>> **p/e**		*Plot error bars*
>> **k/h**		*Keep a hardcopy*
>> **j post11**		*Print on the HET laser printer*
>> **@g:precis**		*Will plot all eight workspace and print them on a single A4 sheet*

6.3. 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 (<1mb)
- ❐ set_ei and cha issued from het$disk0:[het.run]
- ❐ Chopper correctly phased (update, ei crpt)
- ❐ Heater on (if necessary)
- ❐ Command file for automatic update and store running

or

- ❐ Overnight command file or batch job running

7. HET Instrument Parameters.

Incident Energy	15-2000meV
Energy Resolution	1-3%
Beam	N9
Moderator	316K H_2O poisoned at 1.5cm
Background Chopper	100, 50 or 25Hz nimonic 8.5m from moderator
Fermi Chopper	10m from moderator, 150-600Hz phased to ISIS pulse ± 0.5μs. Several chopper packages available optimised for different incident energies.
Sample position	11.82m from moderator
Beam size	4.5cm by 4.5cm
Detectors	3°-7° 4m bank: 52 10atm ^{3}He in four fold azimuthally symmetric array. 9°-29° 2.5m bank: 256 10atm ^{3}He in eight fold azimuthally symmetric array. 110°-125° 4m bank:44 10atm ^{3}He. 130°-140° 2.5m bank:44 10atm ^{3}He.
Monitors	Monitor 1: incident beam monitor Monitor 2:-1.615m from sample Monitor 3: +5.694m from sample
Intensity at sample	$3.3x10^3$n cm^{-2} s^{-1} at Ei=1eV (for 150μAmps proton current)
Sample environment	All standard sample environment equipment
Data acquisition	VAX station 3600

8. HET Detector Angles.

4m low angle bank **d=4.047m**

East			North			West			South		
spec.	det.	angle	*spec.*	det.	angle	*spec.*	det.	angle	*spec.*	det.	angle
1	301	2.59	*21*	315	2.59	*41*	329	2.59	*61*	343	2.59
2	302	2.97	*22*	316	2.97	*42*	330	2.97	*62*	344	2.97
3	303	3.36	*23*	317	3.36	*43*	331	3.36	*63*	345	3.36
4	304	3.74	*24*	318	3.74	*44*	332	3.74	*64*	346	3.74
5	305	4.13	*25*	319	4.13	*45*	333	4.13	*65*	347	4.13
6	306	4.51	*26*	320	4.51	*46*	334	4.51	*66*	348	4.51
7	307	4.90	*27*	321	4.90	*47*	335	4.90	*67*	349	4.90
8	308	5.29	*28*	322	5.29	*48*	336	5.29	*68*	350	5.29
9	309	5.67	*29*	323	5.67	*49*	337	5.67	*69*	351	5.67
10	310	6.06	*30*	324	6.06	*50*	338	6.06	*70*	352	6.06
11	311	6.44	*31*	325	6.44	*51*	339	6.44	*71*	353	6.44
12	312	6.83	*32*	326	6.83	*52*	340	6.83	*72*	354	6.83
13	313	7.21	*33*	327	7.21	*53*	341	7.21	*73*	355	7.21

4m high angle bank **d=4.039m**

Right			Left		
spec.	det.	angle	*spec.*	det.	angle
403	4103	110.42	*453*	4203	110.42
404	4104	110.90	*454*	4204	110.90
405	4105	111.28	*455*	4205	111.28
406	4106	111.70	*456*	4206	111.70
407	4107	112.12	*457*	4207	112.12
408	4108	112.56	*458*	4208	112.56
409	4109	113.02	*459*	4209	113.02
410	4110	113.42	*460*	4210	113.42
411	4111	113.86	*461*	4211	113.86
412	4112	114.28	*462*	4212	114.28
413	4113	114.74	*463*	4213	114.74
414	4114	115.22	*464*	4214	115.22
415	4115	115.60	*465*	4215	115.60
416	4116	115.98	*466*	4216	115.98
417	4117	116.40	*467*	4217	116.40
418	4118	116.80	*468*	4218	116.80
419	4119	117.22	*469*	4219	117.22
420	4120	117.64	*470*	4220	117.64
421	4121	118.10	*471*	4221	118.10
422	4122	118.54	*472*	4222	118.54
423	4123	119.00	*473*	4223	119.00
424	4124	119.44	*474*	4224	119.44

2.5m low angle bank d=2.512m

West			Southwest			South			Southeast		
spec.	det.	angle	*spec.*	det.	angle	*spec.*	det.	angle	*spec.*	det.	angle
101	129	9.31	*133*	161	9.31	*165*	193	9.31	*197*	225	9.31
102	130	9.94	*134*	162	9.94	*166*	194	9.94	*198*	226	9.94
103	131	10.56	*135*	163	10.56	*167*	195	10.56	*199*	227	10.56
104	132	11.19	*136*	164	11.19	*168*	196	11.19	*200*	228	11.19
105	133	11.81	*137*	165	11.81	*169*	197	11.81	*201*	229	11.81
106	134	12.44	*138*	166	12.44	*170*	198	12.44	*202*	230	12.44
107	135	13.06	*139*	167	13.06	*171*	199	13.06	*203*	231	13.06
108	136	13.69	*140*	168	13.69	*172*	200	13.69	*204*	232	13.69
109	137	14.31	*141*	169	14.31	*173*	201	14.31	*205*	233	14.31
110	138	14.94	*142*	170	14.94	*174*	202	14.94	*206*	234	14.94
111	139	15.56	*143*	171	15.56	*175*	203	15.56	*207*	235	15.56
112	140	16.19	*144*	172	16.19	*176*	204	16.19	*208*	236	16.19
113	141	16.81	*145*	173	16.81	*177*	205	16.81	*209*	237	16.81
114	142	17.44	*146*	174	17.44	*178*	206	17.44	*210*	238	17.44
115	143	18.06	*147*	175	18.06	*179*	207	18.06	*211*	239	18.06
116	144	18.69	*148*	176	18.69	*180*	208	18.69	*212*	240	18.69
117	145	19.31	*149*	177	19.31	*181*	209	19.31	*213*	241	19.31
118	146	19.94	*150*	178	19.94	*182*	210	19.94	*214*	242	19.94
119	147	20.56	*151*	179	20.56	*183*	211	20.56	*215*	243	20.56
120	148	21.19	*152*	180	21.19	*184*	212	21.19	*216*	244	21.19
121	149	21.81	*153*	181	21.81	*185*	213	21.81	*217*	245	21.81
122	150	22.44	*154*	182	22.44	*186*	214	22.44	*218*	246	22.44
123	151	23.06	*155*	183	23.06	*187*	215	23.06	*219*	247	23.06
124	152	23.69	*156*	184	23.69	*188*	216	23.69	*220*	248	23.69
125	153	24.31	*157*	185	24.31	*189*	217	24.31	*221*	249	24.31
126	154	24.94	*158*	186	24.94	*190*	218	24.94	*222*	250	24.94
127	155	25.56	*159*	187	25.56	*191*	219	25.56	*223*	251	25.56
128	156	26.19	*160*	188	26.19	*192*	220	26.19	*224*	252	26.19
129	157	26.81	*161*	189	26.81	*193*	221	26.81	*225*	253	26.81
130	158	27.44	*162*	190	27.44	*194*	222	27.44	*226*	254	27.44
131	159	28.06	*163*	191	28.06	*195*	223	28.06	*227*	255	28.06
132	160	28.69	*164*	192	28.69	*196*	224	28.69	*228*	256	28.69

2.5m low angle bank d=2.512m

West			Southwest			South			Southeast		
spec.	det.	angle	*spec.*	det.	angle	*spec.*	det.	angle	*spec.*	det.	angle
229	1	9.31	*261*	33	9.31	*293*	65	9.31	*325*	97	9.31
230	2	9.94	*262*	34	9.94	*294*	66	9.94	*326*	98	9.94
231	3	10.56	*263*	35	10.56	*295*	67	10.56	*327*	99	10.56
232	4	11.19	*264*	36	11.19	*296*	68	11.19	*328*	100	11.19
233	5	11.81	*265*	37	11.81	*297*	69	11.81	*329*	101	11.81
234	6	12.44	*266*	38	12.44	*298*	70	12.44	*330*	102	12.44
235	7	13.06	*267*	39	13.06	*299*	71	13.06	*331*	103	13.06
236	8	13.69	*268*	40	13.69	*300*	72	13.69	*332*	104	13.69
237	9	14.31	*269*	41	14.31	*301*	73	14.31	*333*	105	14.31
238	10	14.94	*270*	42	14.94	*302*	74	14.94	*334*	106	14.94
239	11	15.56	*271*	43	15.56	*303*	75	15.56	*335*	107	15.56
240	12	16.19	*272*	44	16.19	*304*	76	16.19	*336*	108	16.19
241	13	16.81	*273*	45	16.81	*305*	77	16.81	*337*	109	16.81
242	14	17.44	*274*	46	17.44	*306*	78	17.44	*338*	110	17.44
243	15	18.06	*275*	47	18.06	*307*	79	18.06	*339*	111	18.06
244	16	18.69	*276*	48	18.69	*308*	80	18.69	*340*	112	18.69
245	17	19.31	*277*	49	19.31	*309*	81	19.31	*341*	113	19.31
246	18	19.94	*278*	50	19.94	*310*	82	19.94	*342*	114	19.94
247	19	20.56	*279*	51	20.56	*311*	83	20.56	*343*	115	20.56
248	20	21.19	*280*	52	21.19	*312*	84	21.19	*344*	116	21.19
249	21	21.81	*281*	53	21.81	*313*	85	21.81	*345*	117	21.81
250	22	22.44	*282*	54	22.44	*314*	86	22.44	*346*	118	22.44
251	23	23.06	*283*	55	23.06	*315*	87	23.06	*347*	119	23.06
252	24	23.69	*284*	56	23.69	*316*	88	23.69	*348*	120	23.69
253	25	24.31	*285*	57	24.31	*317*	89	24.31	*349*	121	24.31
254	26	24.94	*286*	58	24.94	*318*	90	24.94	*350*	122	24.94
255	27	25.56	*287*	59	25.56	*319*	91	25.56	*351*	123	25.56
256	28	26.19	*288*	60	26.19	*320*	92	26.19	*352*	124	26.19
257	29	26.81	*289*	61	26.81	*321*	93	26.81	*353*	125	26.81
258	30	27.44	*290*	62	27.44	*322*	94	27.44	*354*	126	27.44
259	31	28.06	*291*	63	28.06	*323*	95	28.06	*355*	127	28.06
260	32	28.69	*292*	64	28.69	*324*	96	28.69	*356*	128	28.69

2.5m High angle bank d=2.516m

Right			Left		
spec.	det.	angle	*spec.*	det.	angle
507	5111	125.44	*557*	5211	125.44
508	5112	126.12	*558*	5212	126.12
509	5113	126.76	*559*	5213	126.76
510	5114	127.42	*560*	5214	127.42
511	5115	128.04	*561*	5215	128.04
512	5116	128.62	*562*	5216	128.62
513	5117	129.30	*563*	5217	129.30
514	5118	129.64	*564*	5218	129.64
515	5119	130.54	*565*	5219	130.54
516	5120	131.20	*566*	5220	131.20
517	5121	131.80	*567*	5221	131.80
518	5122	132.48	*568*	5222	132.48
519	5123	133.08	*569*	5223	133.08
520	5124	133.72	*570*	5224	133.72
521	5125	134.36	*571*	5225	134.36
522	5126	134.94	*572*	5226	134.94
523	5127	135.58	*573*	5227	135.58
524	5128	136.26	*574*	5228	136.26
525	5129	136.88	*575*	5229	136.88
526	5130	137.52	*576*	5230	137.52
527	5131	138.12	*577*	5231	138.12
528	5132	138.72	*578*	5232	138.72

9. Eating and Drinking

9.1. RAL Opening Hours

R22 Restaurant

	Mon - Fri	**Sat - Sun**
Breakfast	7.00 - 8.00	8.00 - 9.00
Lunch	11.45 - 13.45	12.00 - 13.00
Dinner	17.00 - 19.00	18.00 - 19.00

R1 coffee lounge	hot drinks/snacks	9.30 - 11.30	(Monday-Friday)
		12.30 - 15.30	"
R22 coffee lounge		12.45 - 13.45	"

9.2. 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

10. Comments/Notes