

PAUL SCHERRER INSTITUTE
Laboratory for Neutron Scattering



Rita II Manual

Version 1.3

LABORATORY FOR NEUTRON SCATTERING

Rita II Manual

Christof Niedermayer and Niels Christensen
Laboratory for Neutron Scattering
Paul Scherrer Institut
CH 5232 Villigen PSI
Phone +41 56 310 2086 • Fax +41 56 310 2989
christof.niedermayer@psi.ch
niels.christensen@psi.ch

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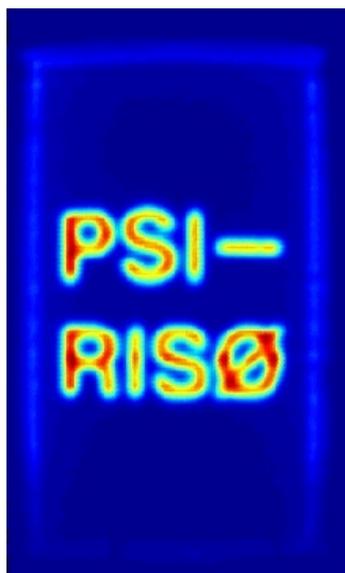
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The Instrument

Rita II is a triple axis spectrometer for cold neutrons at the Swiss Spallation Neutron Source SINQ at the Paul Scherrer Institute in Villigen, Switzerland. The instrument is being operated in a joint venture between the Paul Scherrer Institute and the RISOE National Laboratory, Denmark. RITA II is based upon the conventional triple-axis idea, optimized in several ways. Its main components are:

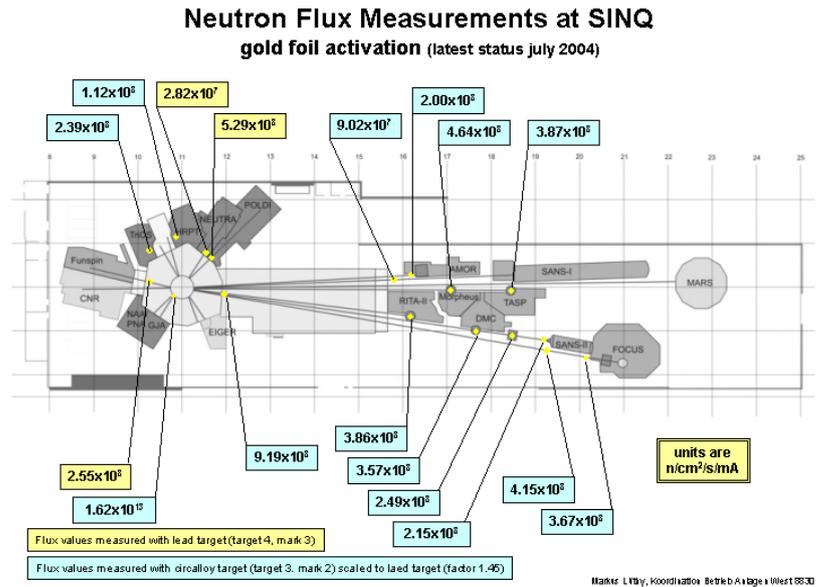
- Supermirror coating ($m=2$) in the neutron beam guide
- A vertically focusing monochromator
- Motorized slits
- Be and BeO filters with built-in collimators
- A flexible 9-bladed analyzer
- A position-sensitive detector (PSD)
- A vertically focusing monochromator

The multi-bladed analyzer combined with the PSD provide flexibility for measurement and opportunities for getting additional efficiency.

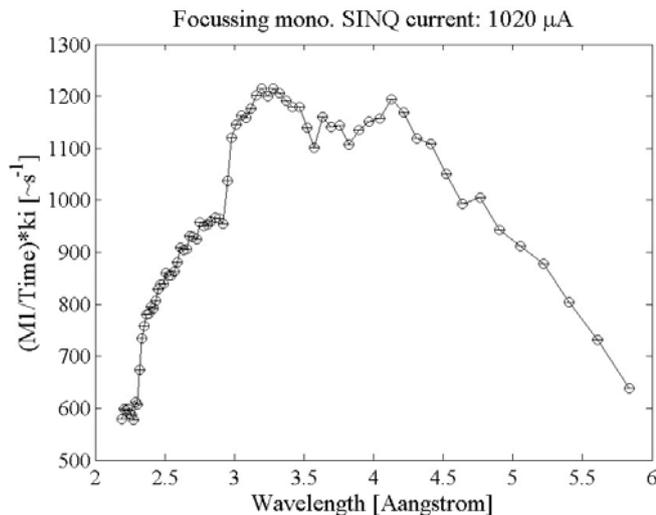


1.1 Beamline and Guide

The neutrons from the Swiss Intense Neutron Source SINQ leave a cold source end enter the guide system RNR13. The primary super mirror ($m=2$) beam guide is 20 m long and has a curvature radius of 2408 m. The guide cross section is $12 \times 3 \text{ cm}^2$. Neutron fluxes were determined by gold foil activation and are given in the figure below.



The SINQ instrument hall at PSI showing the neutron beam line from the source through the guides to the spectrometers. RITA2 is located at the position of the former Drüchhal triple axis spectrometer. The flux measured by gold foil activation is also shown.



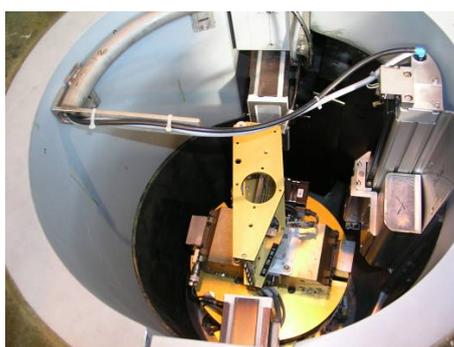
Intensity versus wavelength given as monitor counts per second.

1.2 Monochromator

The RITA II monochromator consists of 5 (vertical) x 3 (horizontal) PG (002) vertically focusing crystals of size 5 cm width * 2.5 cm height. The mosaicity is 40' in both directions. The curvature of the monochromator is controlled by the motor CUM, which turns the blades. The turning of the blades is given by CUM (in arbitrary units) for blade 2 and 4, twice that amount for blade 1 and 5. The optimal curvature depends on the spectrometer energy (see chapter 2).

The proper curvature is automatically set by most scan files. The translations of the monochromator are TUM (in arbitrary units) and TLM (in arbitrary units). The monochromator goniometer is GM.

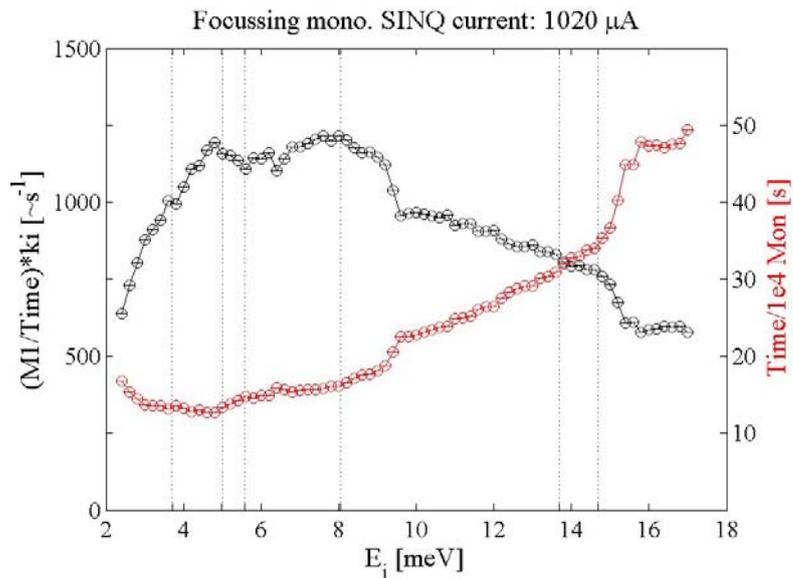
The monochromator is rotated by the motor OMM (or A1, all angles in units of degrees). The corresponding scattering angle is 2TM (or A2). There is an encoder on this angle. The monochromator d – spacing is set by the variable DM (3.354 Å for PG 002).



1.3 Beam Monitor

RITA II is equipped with a ^3He beam monitor with an opening of $80 \times 40 \text{ mm}^2$. This is normally located on a holder on the first motorized slit, right at the exit of the monochromator shielding. The monitor counts are stored in the SICS variable **MON**, and the corresponding rate meters are called **RmS**, **RmM** and **RmF** for slow, medium and fast response times, respectively. The units are counts/sec. Normal monitor count rates are given in the following table.

Configuration									
Seconds per 1000 Monitor									



Measuring time for 10000 Monitor.

1.4 Sample Table

The centre of the sample table is placed 1.406 m from the monochromator axis. This table is designed to hold one of Risø's cryostats or magnets, see the page about the auxiliary equipment. Alternatively, an open-air sample holder, a monitor holder, or an Eulerian cradle may be put on the table. The maximum dimensions for cryostats on the sample table are approximately given by the Risø 9 T magnet: height 150 cm, diameter 44 cm, weight 450 kg. The sample table is shown in Fig. 1.



Figure 1: Pictures of the sample table at the RITA II spectrometer.

The sample table is rotated by the motor OM (A3); the corresponding 2θ angle is called 2T (A4). The maximum movement of 2T is limited by the neutron guide and hence depends on the value of 2TM as given in the following table:

Energy (meV)	3.7	5	13.68	14.7
2TM	89.0	74.16	42.76	41.18
Maximum in 2T	-118	-115	-90	-81

Above the turning plate, there are two translations motors (TU and TL, in units of mm), and above these are two goniometers, GU and GL (measured in degrees).

The height from the top of the sample table to the beam centre is 110 mm. Cryostats, magnets, and open-air sample holders are constructed so that the height from the sample mount to the beam is 57 mm.

1.5 Motorized slits

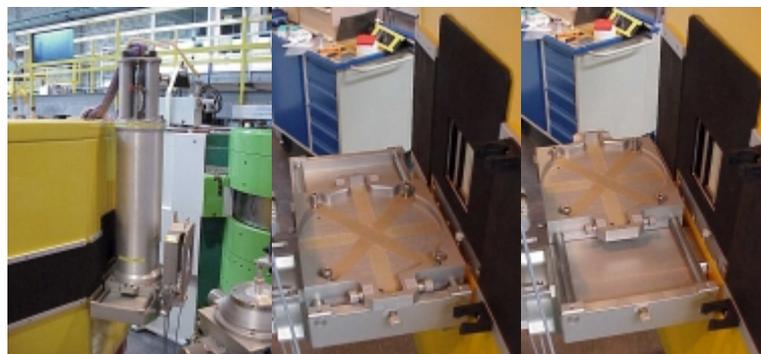
There are four optical benches: Before and after the sample and inside the analyzer tank before and after analyzer. Each can hold a motorized slit. The slits are made from four 10 mm thick BN plates which attenuate the beam by more than 4 orders of magnitude. Each of the four plates has a motor connected. For the monochromator slit the motor names are MSL, MSR, MSB and MST (the third letter denotes left, right, bottom, and top, respectively). The slits after the sample are SSL, SSR, SSB and SST. The analyzer slit motors are named ASL, ASR, ASB and AST and the detector slit motors are DSL, DSR, DSB and DST. All eight motor values are in units of mm.



Neutron monitor and motorized slit after the monochromator.

1.6 Filters

RITA II has two radially collimating filters - a Be and a BeO filter. The filters are meant to be placed right before the analyzer tank, to filter out elastically scattered neutrons in an inelastic experiment. The filters are placed on a special holder and can easily be drawn in or out of the neutron beam. The filters are cooled with liquid nitrogen and have a hold time of 36 h when pumped out well. The filters have to be aligned. The rotation angles are **4 degrees for the BeO filter** (marked on the filter support) and **0 degrees for the Be filter**.



Pictures of the BeO filter and the filter support. The filter can easily be pushed into or out of the beam.

1.7 Analyzer

1.7.1 The analyzer tank

The tank housing the whole analyzer/detector system is shown in fig. 1. The outer walls are made from a mixture of polyethylene and boric acid, and the inside of the stainless steel tank is covered with 5 mm boron-containing plastic. This construction minimizes the neutron background, as most of the fast neutrons are thermalized by hydrogen in the thick walls, while thermal and cold neutrons are absorbed by the boron nuclei.

The walls have an Al opening where neutrons scattered at the sample enter the tank. Here a collimator may be inserted.

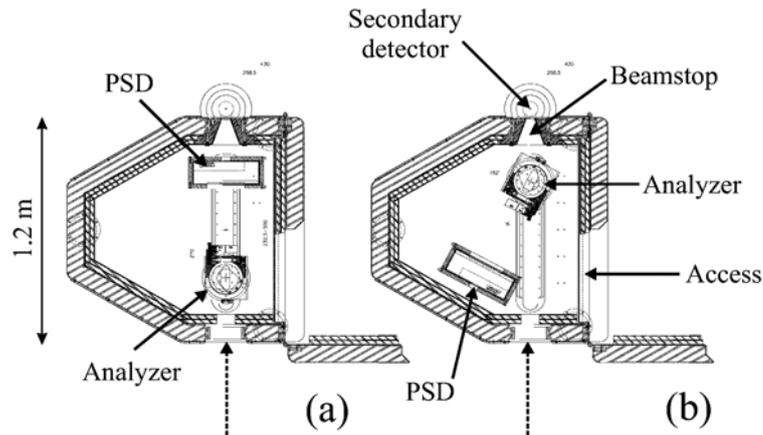


Figure 1: Sketch of the RITA2 analyzer tank.

For monitoring the equipment inside the tank, a small video camera is placed inside the tank and the output is displayed on a video monitor on the control platform.

Entrance to the tank is easy accessible by opening the tank doors, see fig. 2. An optional front shielding is shown on the figure too. Further additional shielding for the inside of the tank is available.

1.7.2 The nine-bladed analyzer

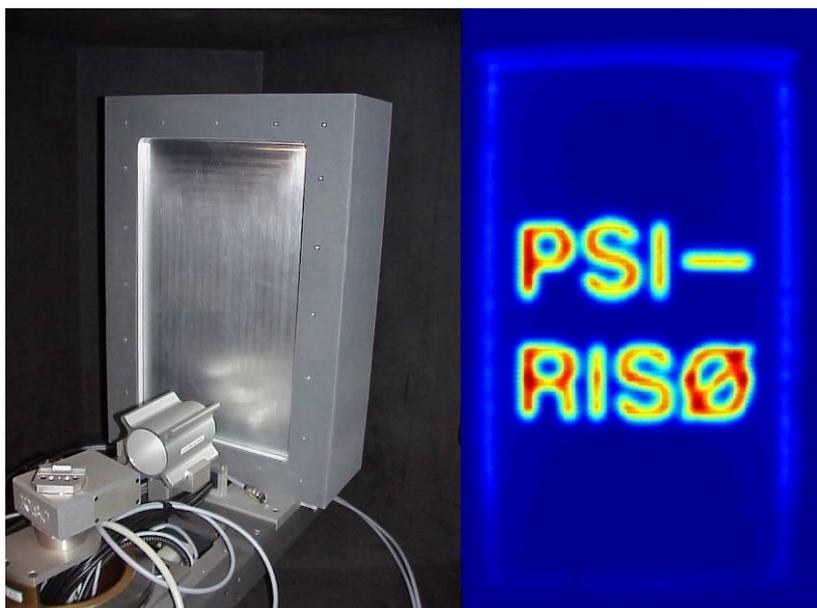
The nine-bladed PG analyzer (at the moment only 7 blades are installed) of the RITA II spectrometer is shown in fig. 3. The blades have the dimensions $24 \times 150 \text{ mm}^2$ and are mounted on vertical axes, each with its own motor. The nine motors are named CA1

through CA9 (where the angle is given in degrees), and they are in turn mounted on an analyzer module with a distance of 25 mm between them. The analyzer axis is located 120.7 cm from the center of the sample table. The analyzer module is also able to rotate around a vertical axis; the corresponding motor is called OMM (A5 when working in one of the standard triple axis modes).

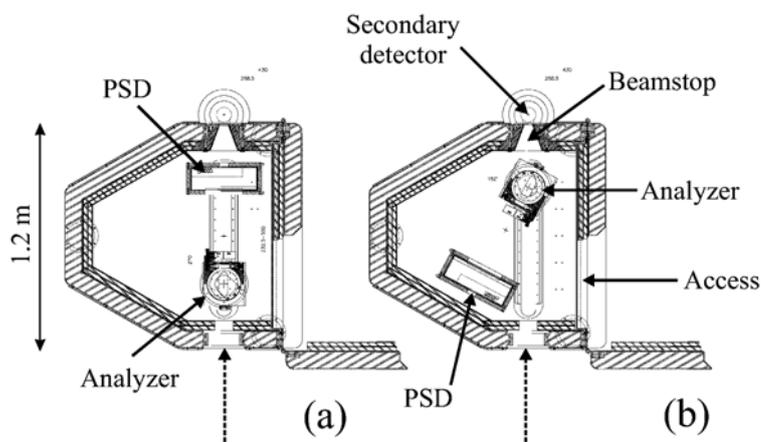
All blades of the analyzer may be set to the same angle by the command PARK a, where a is the setting angle, i.e. a flat analyzer is obtained by typing PARK 0. As for the monochromator, the d-spacing of the reflection at the analyzer must be stated, this is done by setting the variable DA (3.354 Å for PG 002).

1.8 Position Sensitive Detector

For counting the neutrons, RITA II uses a 30x50 cm² position-sensitive detector (PSD), which bins the neutron counts into 128 x 128 pixels, see fig. 1. The distance from the analyzer axis to the detector face is variable and the maximum value depends on the position of the analyzer. The detector is able to swing around in the tank to one side only, see fig. 2. The corresponding motor name is 2TA (A6).



THE INSTRUMENT



Short User Manual

In this chapter we will give a brief introduction into the SING Instrument Control System SICS and the most relevant commands needed to control the instrument during an experiment.

Convention for type-setting in this manual:

- `<device>` stands for all drivable variables (motors, fields, temperatures, etc.)
- `<value>` stands for a required variable entry
- `[<value>]` stands for an optional variable entry
- entrances marked with **SICS** are meant to be written in the command line in the SicsClient
- entrances marked with **term** are meant to be written on the console (e. g. in a xterm)

2.1 Introduction to SICS

SICS (SING Instrument Control System) is a client-server system that controls all neutron spectrometers of SING. There is a magic server program running on the instrument computer which does all the work. The user interacts with SICS only with client applications which communicate with the server through the network. Most instrument hardware (motor controllers, counter boxes etc.) is connected to the system through RS-232 serial connections. These RS-232 ports are connected to a terminal server which is accessed through another server program, the SerPortServer program, which is also running on the instrument computer. The SICS server communicates with the terminal server and other devices through the network. The program was written by Mark Koennecke and a detailed description can be found in the SICS manual.

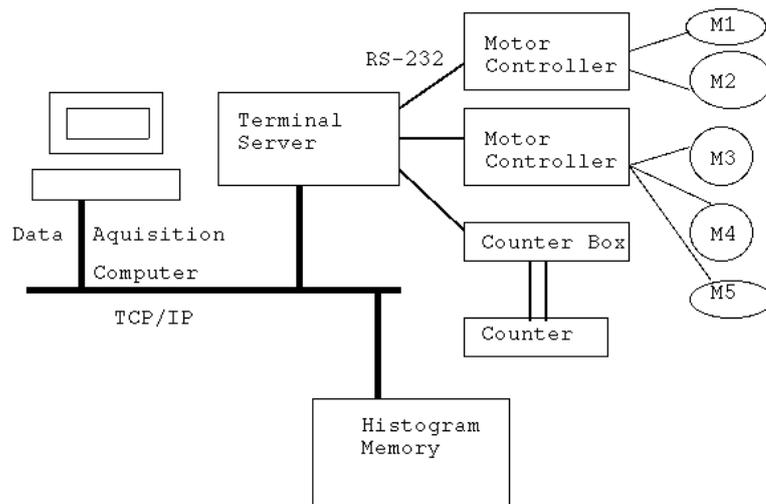


FIGURE 1.1 Hardware Setup at SINQ

2.1.1 RITA-2 Configuration

pc4345, rita2	Instrument computer, running Linux
lnspib01	TCP/IP-GPIB bridge
psts216	Terminal server. All ports configured 9600,8,1,no parity, no flow control, if not stated otherwise.
Ports:	
port 2	EL734 motor controller
port 3	Risø temperature log
port 7	Lakeshore temperature controller



2.2 Starting SICS

1. Check, if the SICServer is running:

```
term ps -A | grep SICS
```

should report at least one line ending with

```
term..... SICServer rita2.tcl.
```

If not, type

```
term startsics
```

For this you'll have to be user rita2 on the computer rita2.psi.ch.

2. Start the SicsClient:

```
term sics&
```

a new window will open.

3. Activate SICS via the pull down menu in the SicsClient:

Connect / RITA2

and

4. Authorize:

Enter User Name and Password

standard user name and password are rita2user and 03lns1

5. Start the status-window:

```
term rita2status &
```

6. Activate the status-window via the pull down menu:

Connect / RITA2

7. An online plot of the PSD can be obtained by

```
term sansstatus &
```

8. Activate the status-window via the pull down menu:

Connect / RITA2

2.2.1 six

six is an alternative to the standard Java SICS commandline client. Why an alternative SICS client?

- It is much faster
- It does not need the X window system
- It connects automatically to the instrument if you are logged into the instrument computer

It has the full functionality of the standard commandline client, but no graphical interface. This means

- you can not (and have not to) use the mouse
- there are no colors to distinguish commands, responses and errors
- instead of clicking on the interrupt button, you have to enter "stop"
- the history is only accessible with the arrow keys

2.3 Drive, Check and Modify device parameters

The current value of a device is reported by just typing its name:

SICS <device>

There are hardware and software limits for all motors. These can be checked for an individual motor by typing

SICS <device> list

To change the software limits type:

SICS <device> softlowerlim <value>, e.g. **SICS** ca5 softlowerlim -200

SICS <device> softupperlim <value>

For PSI motors and encoded RISOE motors (2t and 2ta) repositioning should be done by the command sp, which changes the softzero value.

SICS sp <device> <value>sp, e.g. **SICS** sp omm 37.07

Repositioning of unencoded RISOE motors can be done by the command

SICS<device> putpos <value>, e.g. **SICS** oma putpos 74.17

(This is however at the present state of development not working properly for all motors)

The hardware limits can not be changed!

Drive a device to a value:

SICS dr[ive] <device> <value>

Drive several devices at the same time:

SICS dr[ive] <device1> <value1> <device2> <value2> [etc.]

2.4. UB Matrix and Crystal Alignment

SICS cell a b c alpha beta gamma

set unit cell constants. If b or c are omitted, the same value as for a is used, if angles are omitted, they are set to 90 degrees. Without arguments, the cell constants are listed.

SICS ref qh qk ql a3 a4 sgl sgu Ei Ef

Make an entry in the list of peaks. For angles and k-values not given, the current motor positions are used. If the given qhkl triple already exists, its list entry is overwritten. If not, a new entry is made. The peak number and the peak data are returned.

SICS addauxref qh qk ql

Add an auxiliary reflection to the list of reflections. A4 is calculated from the cell constants, the current ei and ef values are used. A3 is left alone or is calculated to have the right angular difference to the previous reflection. Using auxiliary reflections is a help during setup of the instrument or in powder mode. The sequence:

SICS ref clear

SICS cell aa bb cc alpha beta gamma

SICS addauxref ax ay az

SICS addauxref bx by bz

SICS makeub 1 2

with ax, ay, az being the first plane vector and bx, by, bz being the second plane vectors creates a UB matrix which allows to drive QE positions and qm. But be aware that a3, sgu and sgl values are still invalid.

SICS ref clear peak

Remove a peak.

SICS ref clear all

Remove all peaks.

SICS ref

List all peaks.

SICS makeub peak1 peak2

Calculate, activate and print out the UB matrix, as well as the peak list with qhkl values calculated back. Peak 1 is used as the main peak, i.e. driving to the angles given for this peak will correspond to a QHKL which may only differ by a scalar factor of about one, if the cell constants are not correct. peak2 is used only for determining the scattering plane.

SICS makeubfromcell

Calculate and activate a UB which has been derived from the cell constants alone. This is useful to get a4 when no reflection has yet been found to calculate a proper UB.

SICS makeauxub qh qk ql

Calculate a UB matrix from the first reflection and an auxiliary second reflection specified through the miller indices qh , qk, ql. The auxiliary reflection will have the same angles as the first reflection, except a3 and a4 will be adjusted to match the requirements from the crystals geometry.

SICS listub

List the UB matrix, the cell constants and all stored reflections.

2.4.1 Example Session

First enter the cell parameters

SICS cell 2.88 2.88 2.88 90 90 90

Define the scattering plane

SICS addauxref 2 0 0

SICS addauxref 0 2 0

SICS makeub 1 2

Calculate and activate a UB which has been derived from the cell constants alone. Drive the instrument to the calculated A4 position.

SICS dr a4 position

Find the peak 2 0 0 and optimize it. Once you are at the maximum:

SICS ref 2 0 0

Peak	QH	QK	QL	A4	A3	SGL	SGU
1	2.00	0.00	0.00	65.31	-87.21	1.25	-5.22

Make an auxiliary UB and drive to the theoretical position for 0 4 4

SICS dr qh 0 4 4

Find the 0 4 4 reflection and optimize. Once you are at its maximum:

SICS ref 0 4 4

Peak	QH	QK	QL	A4	A3	SGL	SGU
1	0.00	4.00	4.00	65.31	-87.21	1.25	-5.22

Show the complete peak list:

SICS ref

Peak	QH	QK	QL	A4	A3	SGL	SGU
1	2.00	0.00	0.00	65.31	-87.21	1.25	-5.22
2	0.00	4.00	4.00	99.45	20.39	4.25	-1.22

Calculate the UB matrix, with 2 0 0 as primary peak and 0 4 4 as secondary peak.

SICS makeub 1 2

```

UB  2.456  0.530 -0.200
    -0.530  2.456 -0.090
    0.200  0.090  2.456
Peak QH  QK  QL  A4  A3  SGL  SGU  QH  QK  QL
1 A  2.00  0.00  0.00  65.31 -87.21  1.25 -5.22  2.03  0.00  0.00
2 B  0.00  4.00  4.00  99.45  20.39  4.25 -1.22  0.02  3.95  4.03

```

The last 3 columns above show the Q values calculated back from the angles.

Drive to the 2 0 0 peak

SICS dr qh 2 0 0

SICS pr A4 A3 SGL SGU

```

A4 = 64.218
A3 = -87.515
SGL = 2.258
SGU = -3.217

```

The value of A4 has changed, because the cell constants do not match the values given for the first peak. The value of A3 has changed by the same reason, and in addition, because the the plane given by 2 0 0 and 0 4 4 is now tilted back into in the scattering plane. For the latter reason SGU and SGL have changed also.

SICS DR QH 3 3 3

SICS PR A4 A3 SGL SGU

```

A4 = 82.516
A3 = -31.215
SGL = 2.258
SGU = -3.217

```

Note that the values for SGL and SGU have not changed. They will not change as long as we stay in the scattering plane (no drives to Q3) and as long as the UB matrix has not changed.

SICS REF 3 3 3

```

Peak QH  QK  QL  A4  A3  SGL  SGU
3   3.00  3.00  3.00  82.32 -31.25  2.26 -3.22

```

SICS MAKEUB C B

```

UB  2.456  0.530 -0.200
    -0.530  2.456 -0.090
    0.200  0.090  2.456
Peak QH  QK  QL  A4  A3  SGL  SGU  QH  QK  QL
1   2.00  0.00  0.00  65.31 -87.21  1.25 -5.22  2.03  0.00  0.00
2 B  0.00  4.00  4.00  99.45  20.39  4.25 -1.22  0.02  3.95  4.03

```

3 A 3.00 3.00 3.00 82.32 -31.25 2.26 -3.22 3.00 3.00 3.00

We have calculated a new UB matrix, based on the peak 3 3 3 as primary and the 0 4 4 as secondary peak. The UB matrix has not changed, as we were already exactly at 3 3 3.

2.4.2 Out Of Plane Operation

This formalism allows to drive out of the scattering plane using the tilt motors of the sample stage. Some cryostats cannot stand this. Therefore driving out of plane can be switched off and on.

SICS TASUB OUTOFPLANE 1

This command switches out of plane operation on.

SICS TASUB OUTOFPLANE 0

This command switches out of plane operation off.

SICS TASUB OUTOFPLANE

lists the current value of the out of plane variable

2.5. Scan command

The scan syntax is like on TASMAD. The general scan command is

```
SICS sc[an] <device> <center> <step> <np> <preset>
```

with the arguments :

<device> any driveable variable, and <center> its center value

<step> any step (d immediately followed by the variable name)

<np> followed by the number of points

<preset> followed by the monitor mn or time ti preset value

The presence of 4 argument parts is mandatory, but the order of the parts is not relevant. For every step variable, the corresponding center value must be given. If no step is given for a center variable, a step 0 is used.

Special cases are the variables QH and Q3 , and their corresponding steps DQH and DQ3 which have 4 or 3 values.

Examples:

```
SICS SC A3 40 DA3 0.1 NP 41 MN 1000
```

orders a scan of A3 around 40 degrees with 20 steps to either side with a step width 0.1 and 1000 counts in the monitor. Alternatively, the preset value time gives the counting time in seconds.

```
SICS sc a3 40 da3 0.1 np 41 ti 1
```

Energy scan (the following two beeing equivalent))

```
SICS SC QH 1 0 0 0 DQH 0 0 0 0.01 NP 5 MN 1000
```

```
SICS SC QH 1 0 0 EN 0 DEN 0.01 NP 5 MN 1000
```

q scan (the following two beeing equivalent))

```
SICS SC QH 1 0 0 0 DQH 0 0.01 0 0 NP 5 MN 1000
```

```
SICS SC QH 1 0 0 0 DQH 0 0.01 0 NP 5 MN 1000
```

The scan uses the value of <device> and the number of counts window 5 as plotting variables in rita2status.

One can also scan multiple motors. For example a $\theta - 2\theta$ scan is performed by the following command:

```
SICS sc a3 40.2 da3 0.1 a4 73.5 da4 0.2 np 41 mn 1000
```

2.6. Other Commands and Procedures

2.6.1 Simulation Mode

For testing batch files or in order to check the movement of the instrument it may be helpful to run SICS in simulation mode. You must then connect to a special simulation SICS server.

Open a new sics client and connect to RITA-2-SIM.

```
term sics &
```

In the simulation server, everything is like in the actual SICS server, except that no hardware is moved, no counts collected and no data file written. There is one specialty, however. The command:

```
SICS sync
```

synchronizes the parameters and limits in the simulation server with those in the instrument.

2.6.2 Batch files

To see the batch file path:

```
SICS exe batchpath
```

To change the batch file path:

```
SICS exe batchpath newpath, e.g. SICS exe batchpath /home/rita2/batch
```

To write a batch file:

Produce a text file with a text editor of your choice (emacs, kate etc)

```
term kate test01.job &"
```

Write the commands directly into the text file, as you would have done at the SICS client.

Save the file in the batch directory defined above

To execute the text file type

```
SICS do test01.job
```

The batch file can not be changed once it is executed. A workaround this limitation is to call another batch file at the end of the file.

Example of a batchfile

```

dr ef 5
ritamode monoim

dr tt 10
wait 600

dr mf=5
title (H,L)scan, E=0.7meV, H=5T
sc qh -0.5 0 0.98 0.7 dqh 0.005 0 0.0072 0 np 41 mn 200000

dr mf=0
title (H,L)scan, E=0.7meV, H=0T
sc qh -0.5 0 0.98 0.7 dqh 0.005 0 0.0072 0 np 41 mn 1e6

title energy scan at (1 0 1), H=0T
sc qh 1 0 1 1.5 dqh 0 0 0 0.1 np 41 mn 2e5

do nextjob.job

```

2.6.3 Counter Box Threshold

To prevent collecting background data in case of no beam or a very low beam a threshold value should be set on the PSI counter-box. (In TASCUM this was done by the command CIBO and setting the threshold manually). The PSI counter-box is now accessible from SICS.

The following commands are available:

```
SICS el737 getthreshold 1
```

reads the current threshold

```
SICS el737 setthreshold 1 <value>
```

sets a new threshold.

Typical values are 20 to 50.

2.6.4 Monochromator Curvature

The curvature of the monochromator is controlled by the motor CUM, which turns the blades. The optimal curvature depends on the spectrometer energy and is given by

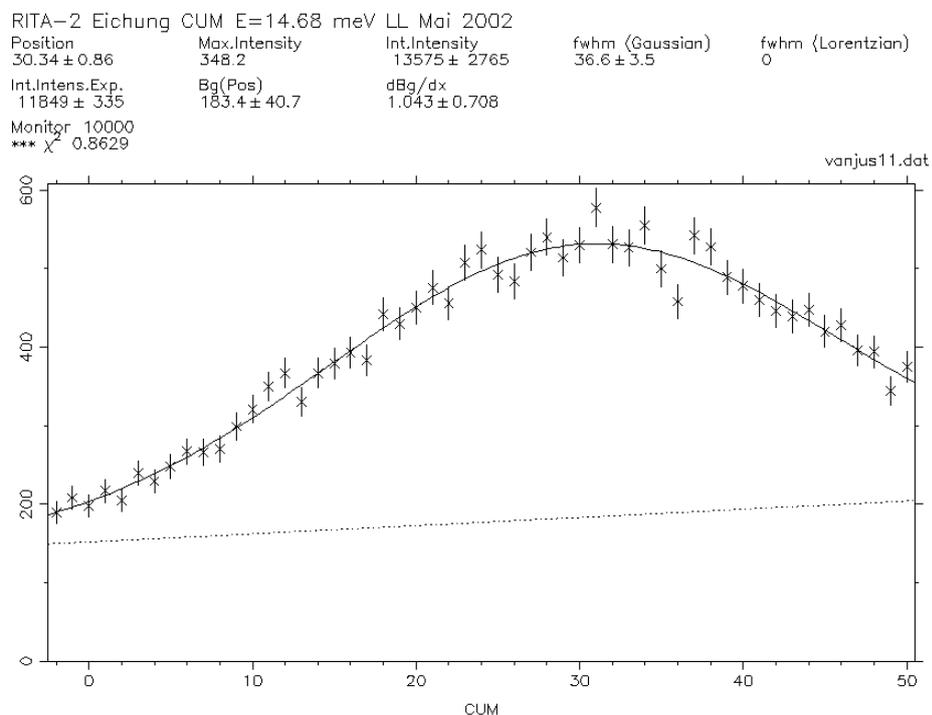
$$CUM = vb1 + vb2 / \sin(omm) \text{ with } vb1 = 0.307 \text{ and } vb2 = 8.90 \text{ (as of April 2007)}$$

These values can be changed by the command

SICS tasub mono vb1 value

SICS tasub mono vb2 value

The gain in intensity compared to a flat monochromator is about 2.5, as can be seen from the figure below.



2.6.5 Scattering Sense

Most experiments are done in a $sm=1$, $ss=-1$ and $sa=1$ configuration, where +1 means scattering to the left and -1 scattering to the right. sm and sa can only be +1, only the scattering sense at the sample can be changed by

SICS se ss value or **SICS** tasub ss value

Rita Modes

Selecting the analyzer mode is an important issue for the RITA II spectrometer. In this chapter we describe the different modes which are available at present for standard operation.

3.1 Two axis and three axis modes

The spectrometer can be run both in two - axis and triple – axis mode.

There are 2 triple-axis modes: ki and kf. (fixed incoming or fixed final energy). Usually the kf option is used.

There is only one 2-axis mode: elastic.

To read which mode the spectrometer is in write

```
SICS tasub const
```

To change the mode write for instance

```
SICS tasub const elastic
```

To avoid a shadow from the edge-on analyzer in two axis mode one may like to turn away OMA (to e.g. 90 degrees) and lock it by

```
SICS fix oma
```

3.2 Flat mode

This mode is selected by the command

```
SICS ritamode flat
```

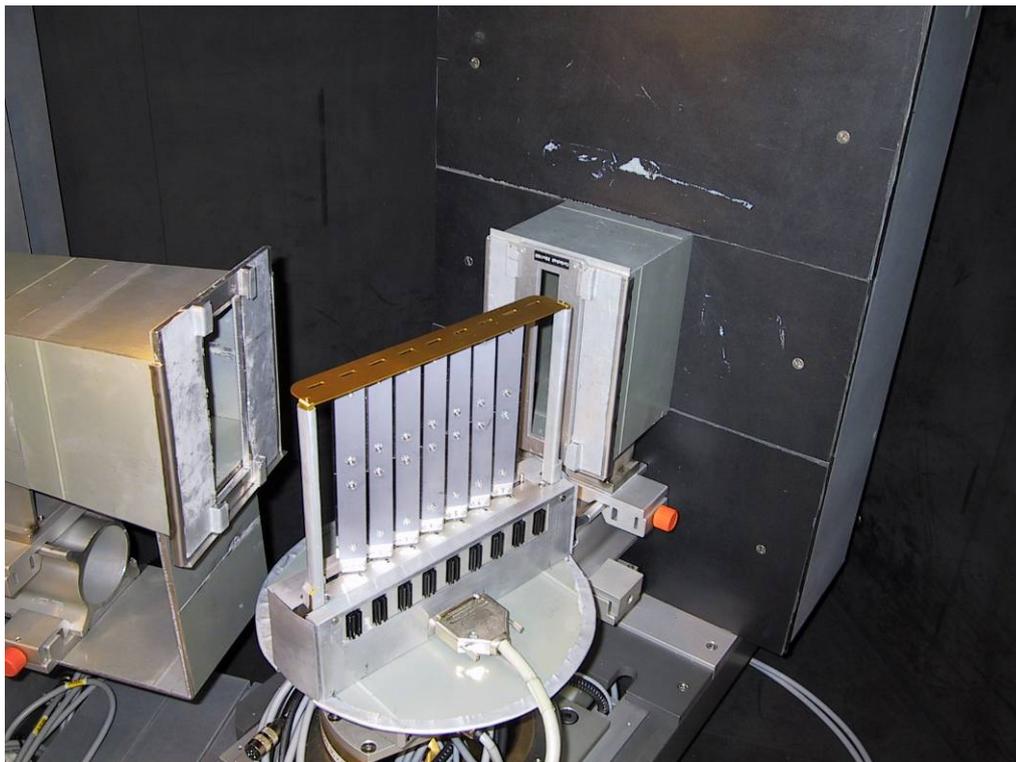
The nine-bladed analyzer is made flat (all cai zero) and oma equal to omm (In standard triple axis notation $A5 = A1$).

3.3 Monochromatic point to point focusing mode

A monochromatic point-to-point focusing mode which produces a reasonable E resolution and a relaxed Q resolution is obtained by

SICS ritamode focus

This mode focuses the beam on the central part of the PSD.



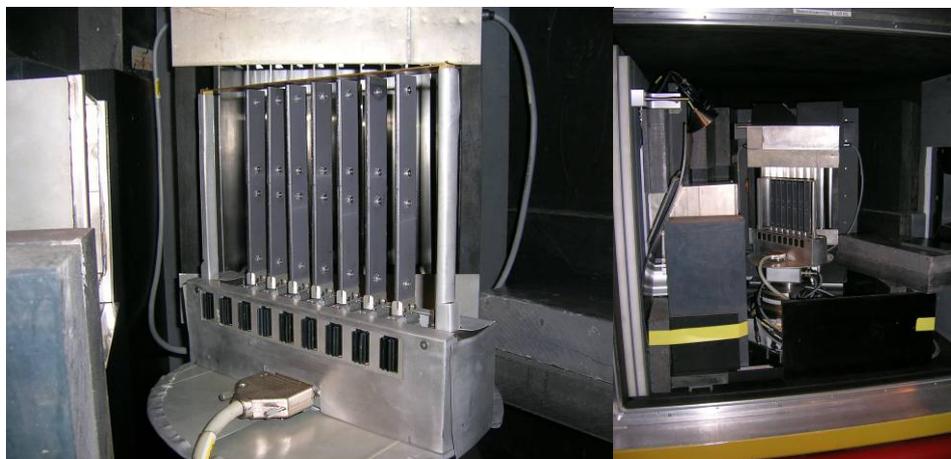
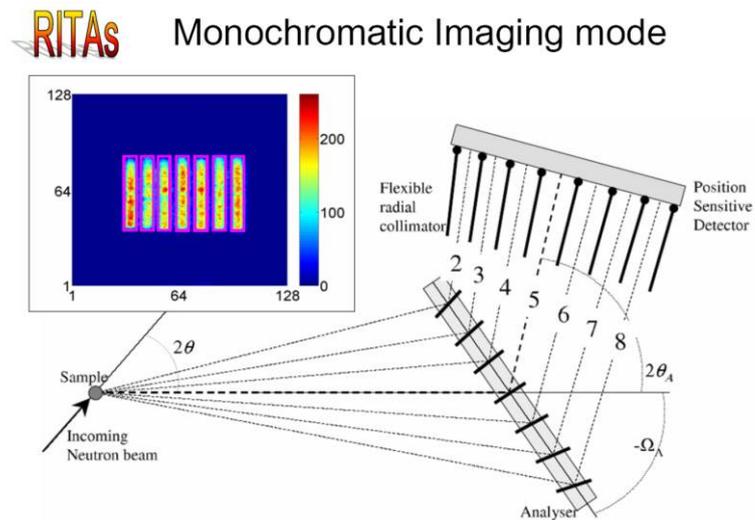
Analyzer configuration in focusing mode. The 7 blades focus the beam on the central part of the PSD. The outer parts of the PSD are covered up by borated polyethylene pieces, which can be screwed to the detector housing.

3.4 Monochromatic imaging mode

The monochromatic q dispersive mode is now fully operational and can routinely be used for experiments. It is obtained by

SICS ritamode monoim

In this mode the different blades scatter on different parts of the PSD and have slightly different q values. In order to minimize cross talk between the blades a flexible radial collimator is installed in front of the PSD.



Analyzer configuration in monochromatic q-dispersive mode.

The collimator blades can be driven by the two motors lc and rc for the left and right half of the collimator, respectively. Typical values for lc and rc are given in the table below:

Ef (meV)	lc	rc
3.7	77	20
5.0	22	0

RITA II Alignment

4.1 Monochromator

- Insert 40' collimator into the beam opening of the monochromator shielding. Place a 15 mm slit in front of the monitor, which is mounted on the 600 mm X95 profile.
- Drive monochromator flat (no curvature)

`SICS` dr cum 0

- Drive A2 (2TM) to the desired value (see Table 1)

Scan (A1) OMM around its nominal value. In order to do this you have to set the counter-box threshold to zero and scan by time (stable beam required)

`SICS` sc omm current_value domm 0.05 np 21 ti 1

find maximum intensity for OMM, drive there and redefine OMM by 2TM/2.

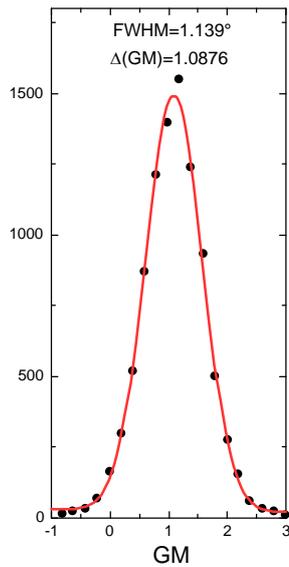
`SICS` sp OMM 2TM/2.

Energy [meV]	Wavelength [Å]	OMM (Θ Monochromator °)	2TM (2Θ Monochromator)
3.63575	4.7434	45.00	90.00
5.0	4.0448	37.08	74.17
8.0	3.1977	28.47	56.94
13.68	2.4453	21.38	42.76

Tabelle 1: Scattering angles A1 (OMM) and A2 (2TM) for specific energies

The monochromator is mounted on a goniometer (motor name GM). Check GM by performing a scan. Before doing so insert a vertical bezel in front of the monitor (vertical opening 30 mm)

`SICS` sc gm current_value dgm 0.1 np 21 mn 1000



Goniometer scan at $E=4$ meV. The measured FWHM is 1.14° and maximum Intensity is obtained at $GM = 1.08$

4.2 2T and neutron energy

Mount the Risø TAS-6 Al_2O_3 sample on the sample table. to determine the neutron energy and the zero point of A4 (2T) (Counting rate in auxiliary detector AUX). Insert a 40' collimator into the analyzer housing. RITA-2 is in 2 axis mode. Measure the intensity of a peak with both negative and positive A4 (2T).

Lazy-Input for Al_2O_3 :

```
TITLE AL2O3
CONDIT      2.4571  5.0 75.0  NE
CELL        4.76100          12.99100  120
SPCRGP R -3 C
ATOM  AL   1  0          0          0.355
ATOM  O    1  0.303    0          0.25
```

```
INTENSITY CALCULATION FOR AL2O3
TRIGONAL STRUCTURE
A= 4.76100, C= 12.99100, WL= 2.45710
```

```
SCATTERING FACTOR COEFFICIENTS
B(AL) = 0.34490 CM-12, B(O) = 0.58030 CM-12
```

Energy [meV]	2Θ (012) d=3.4811 Å	2Θ (104) d=2.5513 Å	2Θ (006) d=2.1652 Å	2Θ (113) d=2.0861 Å	2Θ (116) d=1.6017
Intensity	84.5	56.9	143.7	693.68	1176.62
3.63575	85.89	-	-	-	
5.0	71.04	104.87	-	-	
8.0	54.68	77.61	95.20	100.07	
13.68	41.13	57.27	68.76	71.76	99.52

Table : Al_2O_3 reflexes at different energies

4.3 Monochromator curvature

Remove the 40' collimator from the analyzer housing. Die Energie der einfallenden Neutronen ist nun bestimmt, was nun optimiert werden kann, ist die Krümmung des Monochromators CUM. SICS uses a macro to calculate the energy dependnet curvature:

$$CUM = A_1 + A_2 \cdot 2 \cdot d_{PG002} \cdot \sqrt{\frac{E}{81.804}} \quad \text{with } A_1=0.44 \text{ und } A_2=10.87$$

The constants A1 and A2 have to be determined experimentally.

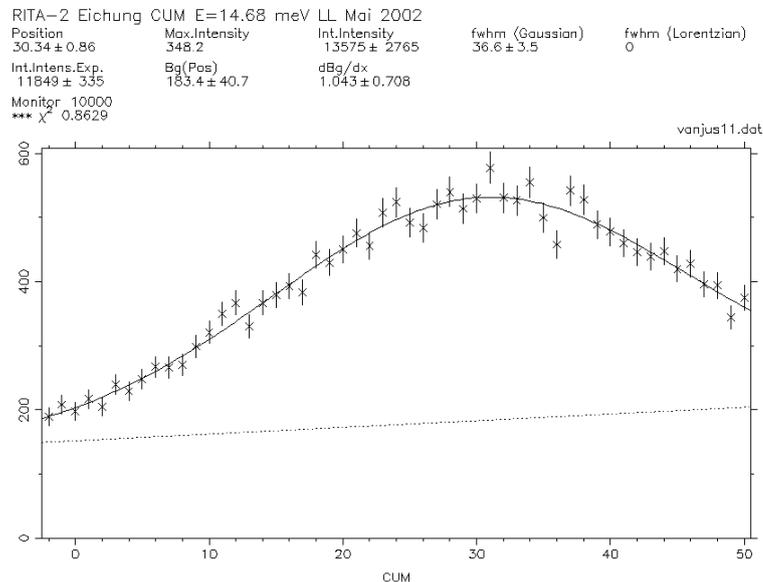
Mount a Vanadium sample. Set A4 to 90 degrees. Perform cum scans at different neutron energies.

SICS dr ef 5

SICS sc cum 26 dcum 1 np 51 mn 1000

SICS dr ef 8

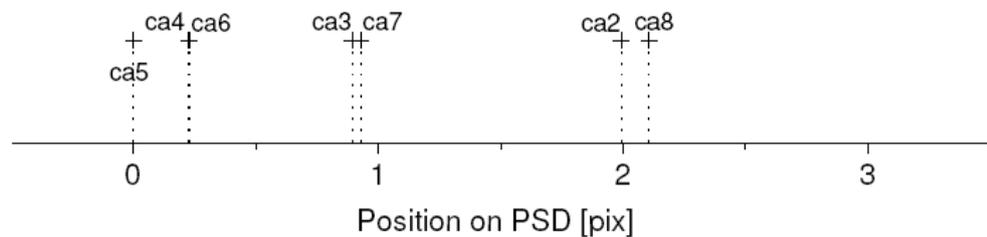
SICS sc cum 26 dcum 1 np 51 mn 1000



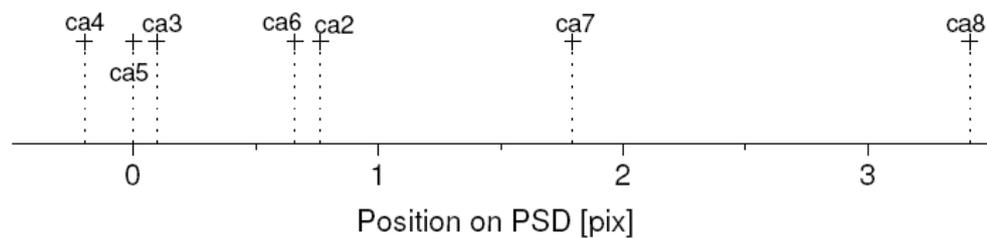
Intensity versus monochromator curvature CUM at $E_f = 14.68$ meV. From the energy dependent maxima $CUM_{\max}(E_f)$ one can determine the SICS - macro parameters A_1 and A_2 .

4.4 OMA calibration

It has for some time been a problem that the angle between the analyzer rack and the beam (motor OMA) cannot be properly calibrated. This is due to the flexibility of the analyzer in the capability of turning the analyzer blades. As the blades turn around the same axes as OMA (certainly blade 5), only one of these angles can be calibrated. The analyzer consists of 7 blades numbered 2 to 8 controlled by the motors ca2 to ca8. The point-to-point focusing mode (ritamode focus) was designed to monochromatically focus the beams reflected from the different blades of the analyzer to the same point on the detector. Because of the asymmetry of the analyzer rack relative to the incoming neutron beam and the asymmetry of the detector to the analyzer, the beams from the different blades will actually intersect the detector at slightly different positions. This is seen in figure 1(a) calculated theoretically, assuming 5 meV neutrons and perfect alignment of all angles.



(a) Perfect alignment of OMA



(b) OMA 2° below perfect alignment

The calculated intersection points on the PSD in the point-to-point focusing mode.

The beam from the central blade (ca5) is defined to intersect the detector at 0. This corresponds to pixel 64 on the PSD. The exact position of the intersection can be controlled with the motor 2TA. Actually this can be used to calibrate 2TA. In the following it is only the relative position of the intersections, that is important. It is seen in figure 1(a), that the rest of the blades intersect the detector nearly pairwise, in distances increasing with the blade distance from the central blade. Plotting these distances from the central blade as a function of blade number gives a parabola, see figures at the end.

If the angle OMA is above or below the perfectly aligned value, the center of the parabola will be shifted, and the intersection of the beams will not be pairwise, see figure 1(b) and the figures at the end.

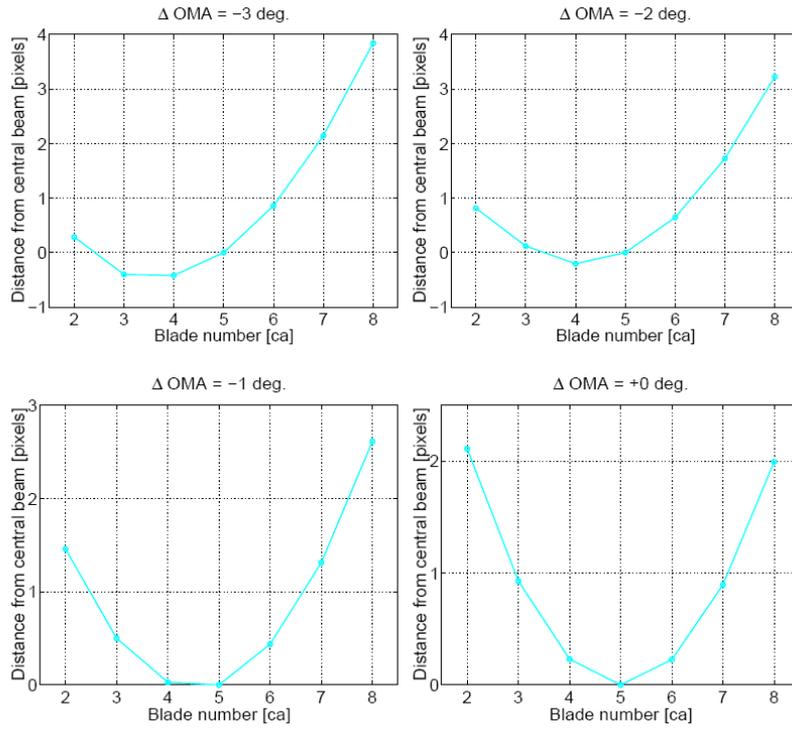
This section will describe alignment of OMA and the analyzer blades using the point-to-point focusing mode. The energy is set to $E_F = 5$ meV, corresponding to $2TA = 74.17^\circ$. First invoke this mode by `ritamode focus`, making sure that all the blades are free to move. Place a vanadium or plastic sample on the sample table.

Run `cascan macro`. This will scan each blade one at a time, leaving the others parked at 0. After each scan a `pixscanx` of the PSD is taken at the most intense position of the blade. This gives the position of the blades reflection on the PSD. The macro gives a table showing the old position, the maximum intensity position and the position on the PSD of each blade.

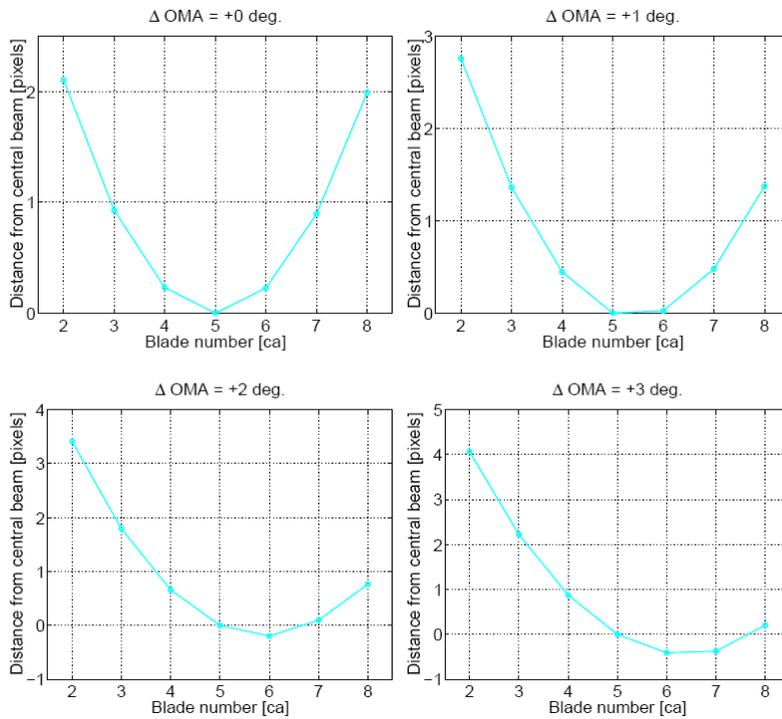
Plot the positions of the blades versus blade number, and connect the points with a parabola. The position of the center of the parabola gives the error in OMA. The figures at the end can be consulted to determine the magnitude of the error.

Now move OMA by subtracting ΔOMA and `remo` to the value it had before. (i.e. if OMA is 74.17° and ΔOMA is found as -2° , set `OMA = 76.17` and `remo` to `74.17`.)

Move the `ca` motors according to the movement in OMA. BUT note that the values of the `ca` motors rise clockwise opposite to all other motors, where the values rise anticlockwise. This means that the `ca`'s must be compensated in the same (numerical) direction as OMA. If the change in OMA angle is considerable (more than 1–2) the blades should be recalibrated with the `cascan macro`, as the asymmetry means that the blades can not be compensated by exactly the same amount as OMA is moved.



Peak position on the PSD for the different blades for a negative ΔOMA ($E_F = 5$ meV).



Peak position on the PSD for the different blades for a positive ΔOMA ($E_F = 5$ meV).

Data Treatment and Analysis

5.1 Data Format

NeXus is a joint effort of both the synchrotron and neutron scattering community to develop a common data exchange format based on a hierarchical data format (HDF). As physical file format the HDF from the National Center for Supercomputing Applications (NCSA) was chosen. This is a binary, platform independent, self describing data format. HDF is well supported by major data analysis packages. HDF files are accessed through a library of access functions. This library is public domain software. Libraries are available for the ANSI-C, Fortran77 and Java programming languages on all important computing platforms.

term hdfview

The screenshot shows the HDFView application interface. On the left is a tree view of the HDF file structure, including paths like 'entry1', 'RITA-2', 'control', 'data', and 'definition'. The main window displays a table of data for the path '/entry1/data/Qh'. The table has 9 columns and 36 rows of numerical data. Below the table, there is a status bar with the following text:

```
HDFView root - /afs/psl.ch/project/sinca/sl-linux/stow/hdfview
User property file - /home/rita2/hdfview2.3
http://hdf.ncsa.uiuc.edu/hdf-java/html/hdfview/UsersGuide/index.html
TableView - /afs/psl.ch/project/sinca/data/2007/rita2/001/rita22007n001258.hdf - /entry1/data/Qh [ dims:9x1, start:0x0, count:43x3, stride:1x1 ]
```

At the bottom, there are buttons for 'Log Info' and 'Metadata'.

5.2 Data Storage

Under the directory `/home/rita2` a directory `data/` exists. In `data/` you will find some directories according to each year (2006/, 2007/,...). Starting from 2006 onwards within the year directory the data files are grouped in subdirectories for each 1000 data files named 001/, 002/, 003, etc. All data files produced are stored in these directories according to the year and number they were obtained. The data files have the general syntax `rita2yearnxxxxxx.hdf` with `xxxxxx` (6 digits) the run number of the file and year the year of production, e.g.:

```
home/rita2/data/2010/001/rita22010n001258.hdf
```

Routinely all new data files are backed up immediately on the machine `lnsa15.psi.ch`, which is accessible through the AFS file system at PSI. Within UNIX environment one has to get access to the directory `root/afs/psi.ch/project/sinqdata/2010/rita2` and then to the desired data subdirectory. From there one can copy files to other disks etc.

```
afs/psi.ch/project/sinqdata/2010/rita2/001/rita22010n001258.hdf
```

5.3 Data Analysis

5.3.1 Data Conversion

You can convert the hdf data into an ASCII file, which you can then import into your favorite data analysis program.

```
term hdf2ascii(`filename`)
```

converts to `filename.asc` in the current directory

5.3.2 Matlab Routines

Log on to the Rita computer

```
term ssh -x rita2@rita2
```

Ask local contact for password.

```
term cd matlab
```

setup the necessary path info in `mypaths`.

Matlab `s=hdf2spec('filename','scanvariable',flag)`

e.g.

`s=hdf2spec('/afs/psi.ch/project/sinqdata/2010/rita2/001/rita22010n001258.hdf','E5',1)`

Creates a 1x7 `spec1d` object.

Flag = 0,1 divides (1) or does not (0) divide by monitor

Matlab `Det_Images('filename')`

e.g.

`Det_Images('/home/rita2/data/2010/001/rita22010n001258.hfd')`

Graphical User Interface

Matlab `qad_view`

`[fs,ps]=fits(s,'gauss',[1 2.4 0.2 0],[1 1 1 1])`

Gaussian fit to `s` with start parameters `[1 2.4 0.2 0]` (Amplitude, Position, width, Background)

Sample Environment Control

6.1. Sample Environment Automation (SEA)

SEA means "Sample Environment Automation". It is a client - server software for controlling and monitoring sample environment devices, such as Lake Shore temperature or Oxford magnet controllers. Its main features include:

- Logging of all relevant variables at 5 sec interval, stored for at least one year
- Control logic not handled by the hardware: automatic needle valve control, correction for sample - heat exchanger difference
- Charts for live display and for inspecting the history
- Graphical user interface for changing control parameters
- Command interface (commands can be used in an instrument batch file, or entered directly)

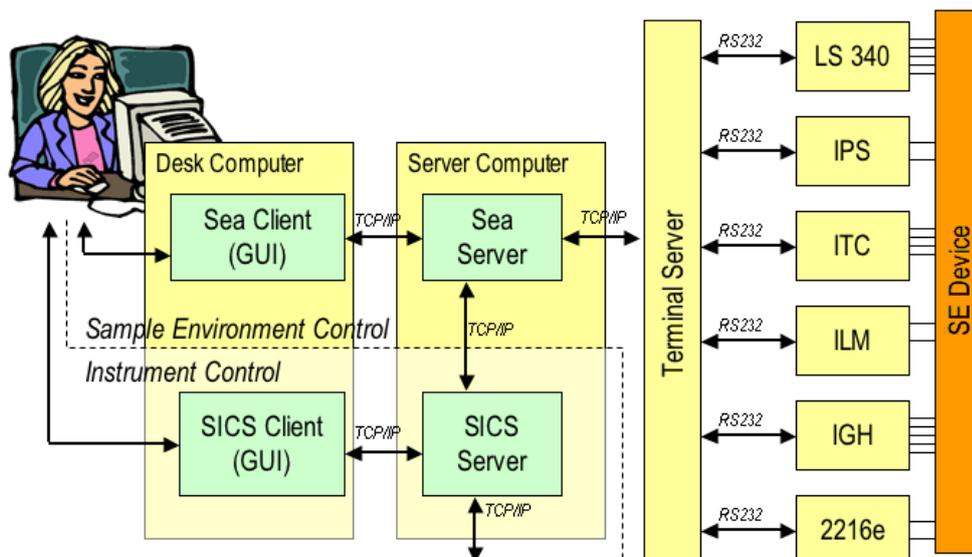
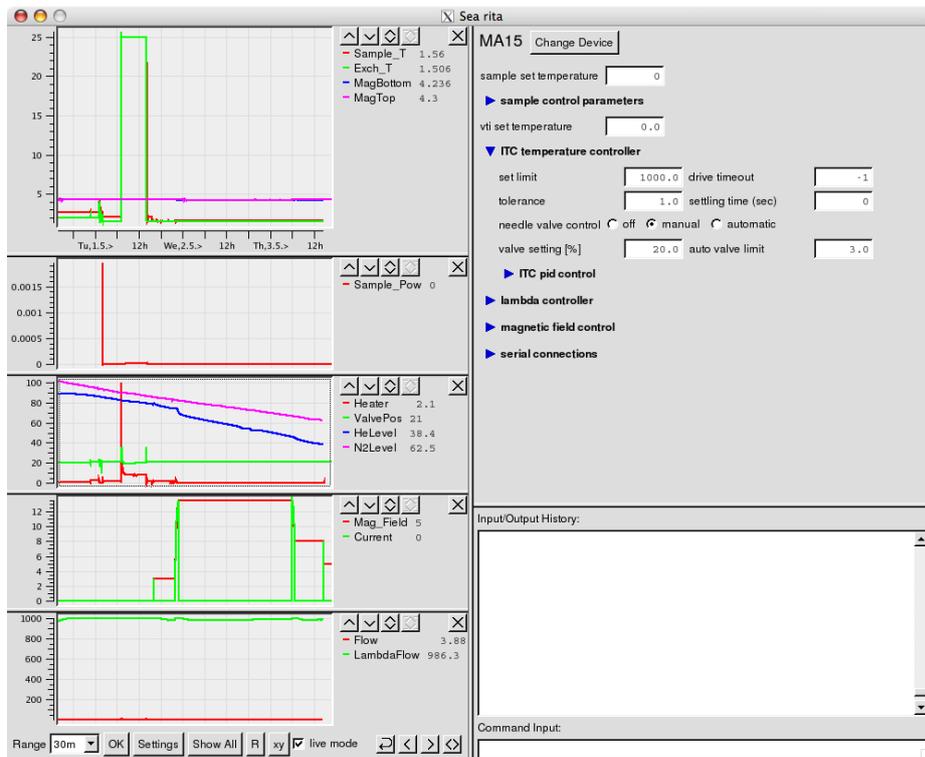


Diagram showing the client - server architecture of SEA and how it is embedded into the instrument control software.

To start a SEA client enter

`term sea &`

on the unix command line, or click on the SEA icon on the linux desktop.



The SEA graphical user interface

Once the sea user interface appears select the cryostat/device in use, if not already done automatically. (e.g. DISE for the Risoe Displex E, MA15 for the 15 T magnet)

In SICS temperatures are changed by:

`SICS run tt 50`

just sets the temperature without waiting, control is given back to sics immediately

`SICS dr tt 50`

waits for temperature to be stable. Stability criteria and settling time can be changed in sea window.

Variable name for magnetic field is mf.

`SICS dr mf 5`

Changes the magnetic field to 5 T on the magnet in use.

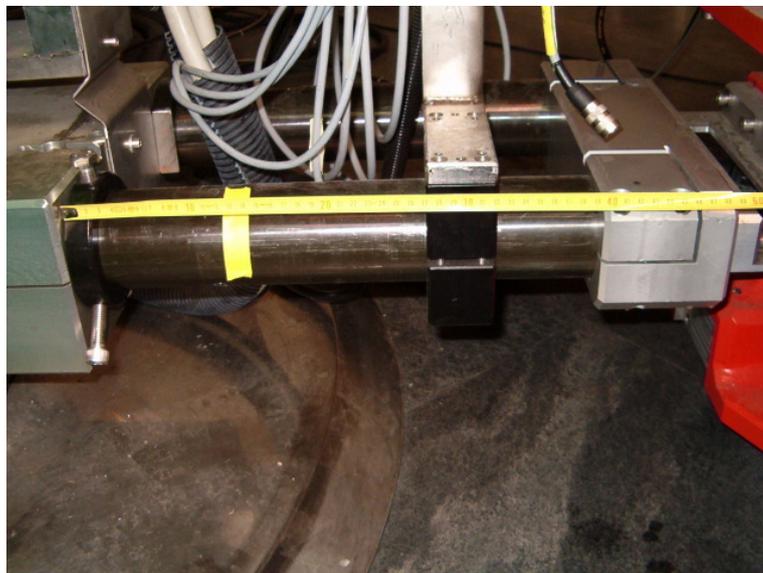
The Oxford 15T magnet MA15

7.1 Regulations and Specifications

The forces on the magnet may not exceed 100 kg. Under normal operation conditions the forces from the monochromator shielding exceed this value and requires an extension of the monochromator – sample distance. The operation of MA15 on Rita-II is thus only allowed for the following conditions:

- * between 3.0 and 17.0 meV at a distance of 450 mm or more, up to 14.9 Tesla
- * between 3.0 and 8.0 meV at a distance of 410 mm or more, up to 13.5 Tesla
- * between 8.0 and 17.0 meV at a distance of 410 mm or more, up to 11.5 Tesla

For any other configuration force tests have to be done.

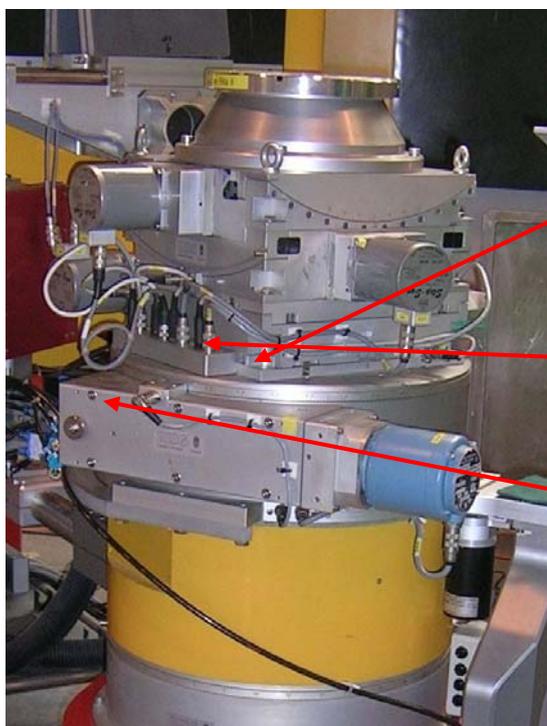


How the distance has to be measured. In this example the distance is around 400 mm.

7.2 Installing MA15

The 15 T magnet requires a completely non magnetic environment. The goniometer motors thus have to be removed and replaced by a rigid support, which does not allow for any tilt. The magnet also does not allow for any rotation. The sample table motor OM (A3) can thus be not used and is replaced by a rotating sample stick .

Remove goniometer from the sample table. Only unscrew the 4 screws connecting the goniometer with the sample table. Do not take the goniometer apart. Unplug the cables for the goniometer and translation motors (see picture below).

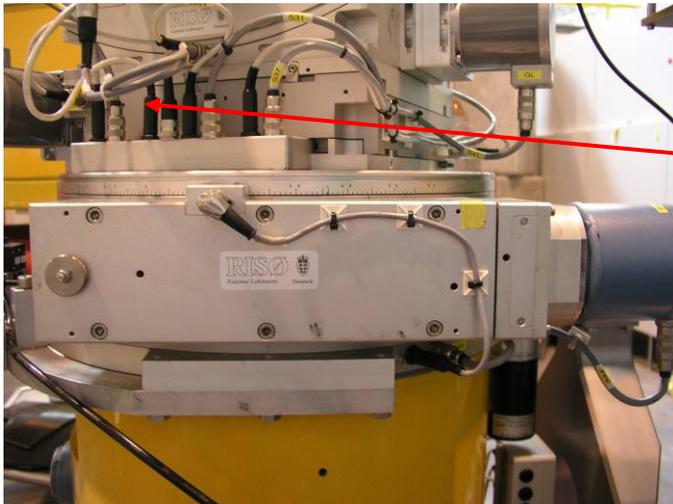


Unscrew here (4 screws)

Unplug cables here

Screws holding omega motor
(6 screws)

THE 15 T VERTICAL MAGNET MA15

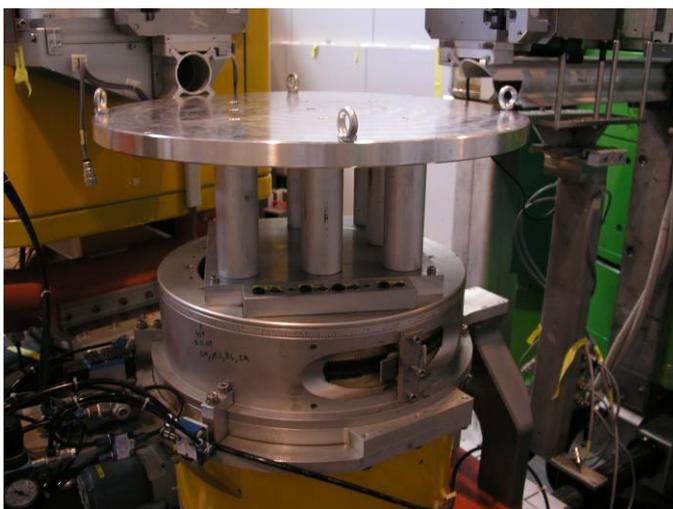


Unplug cables here

Replace the 4 limit switch plugs by dummy plugs to prevent the ECB system from crashing.



Mount the MA15 socket.



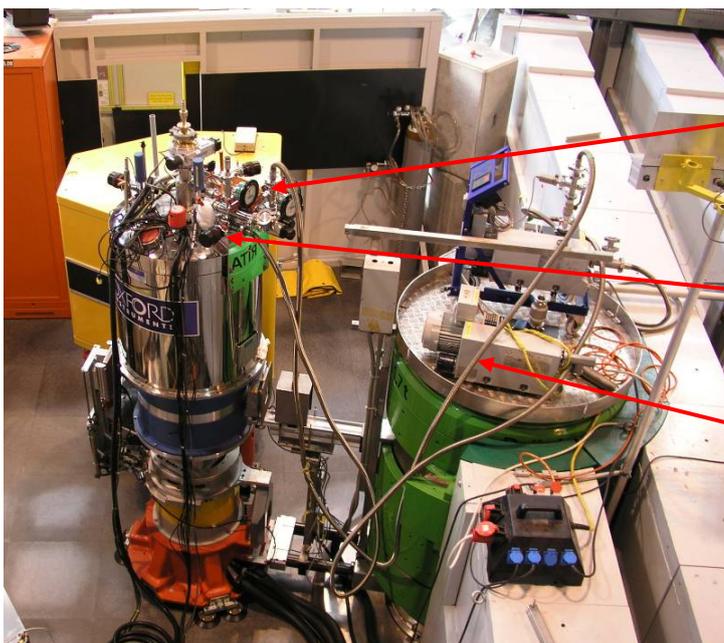
Install the magnet. Matching plugs and sockets are marked with the same color.



Motor Controller for Sample Rotation



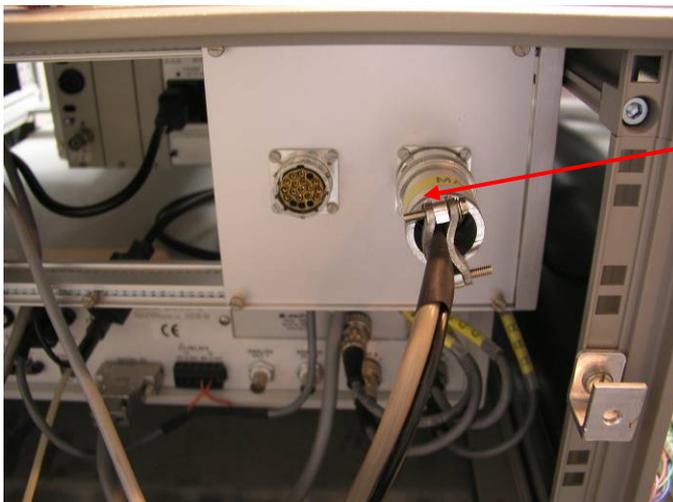
Current Leads for magnet



VTI (to He pump)

Helium Recovery Line

He pump for Lambda stage for fields above 13.5 T.



Connect sample temperature cable with the Lakeshore Controller.

Connect all the other cables according to the color scheme.

RITA2 Serial Connections

Lantronix Terminal Server Insts02.psi.ch

Chan	Cable	Description
1		service channel (reserved)
2		PSI motor controller EL734 (monochromator motors)
3		
4		mobile PSI motor controller EL734 (omega motor on MA15 sample stick)
5		PSI counter box EL737
6		
7		LakeShore 340
8		
9		Needle Valve Controller
10		ILM Oxford Instruments Level Meter (2 stop bits)
11		IPS Oxford Instruments Magnet Power Supply (2 stop bits)
12		IGH Oxford Instruments Gas Handling System (2 stop bits)
13		Oxford Instruments lambda controller (2 stop bits)
14		ITC Oxford Instruments Temperature Controller (2 stop bits)
15		LakeShore 370 (7 bit, odd parity)
16		

The MA15 entrance window is defined by a line marked as WINDOW CENTER LINE. Line up this line with the monochromator - sample axis. This is most easily done by aligning the 45° mark with the 45° mark on the sample table angle scale (or 135°, 225°, 315°).



7.3 Change to / from Omega Motor on Sample Stick

in /home/rita2/rita2_sics/rita2.tcl change the following line

set ma15motor 1 (1 for motor on sample stick, 0 for normal omega table)

and then restart sics with the command

```
term monit restart sicsserver
```

If the motor is not running, it may be necessary to load the motor parameters with the el734_test program. Type

```
term el734_test -help
```

for documentation. A parameter file can be found under /home/users/tascom/PSI/mot_4_01.par

The serial cable for the omega motor is connected to channel 4 (port 3004) on the terminal server lnsts02.psi.ch.

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