THE IMS1270 CIPS USER'S MANUAL (1)
Starting and Running the instruments

Customizable Ion Probe Software

Version 4.0

*CIPS User's Manual (1), June 2003, not fully documented for the section **Other Analysis***

CONTENTS

end of contents

1. Introduction

1.1 The IMS1270 documentation

The IMS1270 documentation consists of:

The IMS 6F/ IMS 1270 User's guide
The IMS1270 dedicated keyboard user's manual, version 98-1
The IMS1270 ion optics User's manual, version 96-1
User's guide for Multicollector release 1.1
IMS6f/1270 Maintenance guide
National Instruments™ LabVIEW® User Manual

This CIPS user's guide consists of 3 parts
 (1) Starting and Running the instruments (This document)
 (2) Processing and tools
 (3) Appendices

1.2 About CIPS

  The CIPS software has been developped by Cameca under the *LabVIEW®* environment (From *National Instruments™*) . It is mainly oriented towards geological applications and isotope ratio analysis.
  The *LabVIEW®* user manual is a part of the documentation delivered with the *LabVIEW* full development version required for the IMS 1270. CIPS users must read the Chapter 16 *Graph and Chart controls indicators*. Some pages of this manual are copied in the appendix *LabVIEW® graph options and graph cursors* in the third part of this CIPS user's guide.

Starting CIPS
* Login
* Display the *openwindows* menu (click in the blue background) and select *CIPS* (A window *CIPS* is then opened)
* Answer *Yes* to the 2 questions which are asked along the installation of CIPS :
"*Do you want to use the back-up holder file ?*"
"*Do you want to use the back-up calibration file ?*"

CIPS scrash
If the program is frozen, type *Ctrl C* in the CIPS window
Restart *CIPS* as explained above.

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1.3 The Server

  Both *SUN™* workstation and microprocessor tasks can communicate between themselves by the mean of a UNIX mailbox process called IPC (Inter Process Communication). The so-called *ServerSun* program insures the message transfer between the *SUN™* workstation and the microprocessor.

Some communication problems may result in server troubles. Possible error messages are:

- *Server generic error* **Continue** *or* **Stop**. It is Highly recommended to click *Continue*.
- *Server Timeout*

If some *CIPS* applications are still scrashed, try to click the small button displayed in the main menu bar, between *TOOLS* and *Exit*.

If clicking the small button fails to re-start the server, open a server window by clicking server in the openwindows menu and type *Ctrl C* in this window.

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1.4 CIPS Overview

The main menu of CIPS consists of a bar containing the following buttons:
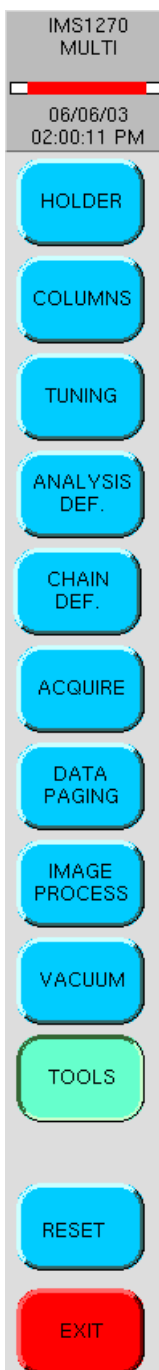
Holder ,Program dedicated to the control of the sample stage motion. It allows to edit, to save and to recall locations of a given sample holder. refer to the CIPS user's manual (2), section § *The stage navigator (Holder)*

Columns Program dedicated to the ion optics save and restore functions. It allows also to run automatic source start and stop procedures. See below the sections § *Saving and restoring Keyboard files* and § *Starting and stopping the source*

Tuning Program dedicated to the instrument setting on, in combination with the keyboard. It allows also to call the *Mass Calibration* program. See below the section § *Checking the instrument before an analysis*

Analysis Definition Program dedicated to the edition of analysis recipes. It allows also to call the *Mass Calibration* program. See the hereunder sections § *Defining an isotope analysis* and § *Other analysis*.

Acquire Program dedicated to run analyses. Analysis results are displayed in real time. It allows also to call the program *Mass Calibration* . See below the section § *Running an analysis*.

Data Paging Program dedicated to the processing of the output analysis data. See below the sections § *Checking the Mass resolution and the peak flatness* and § *Displaying and processing the Isotope analysis results* in the *user's manual (2)*.

Image Process Program dedicated to the processing of scanning ion images. See the section § *Image Processing* in the *user's manual (2)*

Vacuum, Interface dedicated for displaying and controlling the Vacuum system. See § *The Vacuum synoptics* in the *user's manual (2)*

Reset to be used when the kbd error message is displayed.

Tools Opens the additional *Tools* menu. See just below.

Exit For closing CIPS

The *Tools* Bar

STABILITY	SETUP	PERIODIC TABLE	PHA
MULTICOL	TEST	More Tools	QUIT

Stability	Direct recording and displaying of any primary or secondary signals. Statistical functions for featuring a recorded stability curve. See the section § *Stability* in the *user's manual (2)*
Set-up	Panels for editing the actual configuration of the implemented hardware. See the section § *The Setup panels* in the *user's manual (2)*
Periodic Table	Displays the Mendeleiev table, allows to select and edit a simple or compound mass. For a given sample, computes all the interferences at the neighbourhood af a given mass. See the section § *Periodic Table* in the *user's manual (2)*
PHA	Program dedicated to the record of the EM Pulse Height distribution. See the section § *PHA* in the *user's manual (2)*
Multicol	Opens the *Multicollection control* panel. See below the section § *The Multicollection control dialog box*.
Test	A set of functions for testing and debugging the hardware. See the section § *Other Tools* in the *user's manual (2)*
More Tools	See the section § *Other Tools* in the *user's manual (2)*
Quit	Closes *CIPS* and Quits

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2. The [M,B] table

2.1 Basics

2.1.1 The relationship between B and M

At a given accelerating voltage (V), the relationship between the magnetic field (B) and the mass (M) is given by the relationship :

$$B^2 = K * k(B) * M * V$$

where K is a constant for a given range (see below, § The IMS1270 four mass ranges) given instrument and k(B) very close to 1 (comprised between 0.96 and 1.04)

At a given accelerating voltage V, approximating k(B) to 1, a single couple values (M,B) may be used to determine K coarsely, but a single point is not sufficient to mass calibrate finely the spectrometer. Practically, as high magnetic fields produce non-uniform pole piece saturation and the magnetic field is measured with a single Hall probe system, k(B) varies slightly over the B range. Therefore, to be accurate, the mass calibration program works with a K*k(B) parameter which is mass range dependent.

A mass calibration procedure consists of establishing a relationship between a given mass and the corresponding magnetic field and of storing the values (M,B) in a mass calibration table.

A mass calibration table consists of :

- The secondary accelerating voltage
- The secondary polarity.
- N values $(M,B)_i$, with $1 < i < 2000$. M_i values are integer numbers.

For every mass interval $[M_i, M_j]$, K_j is computed following :

$$K_j = (B_j^2 - B_i^2) / (M_j - M_i)$$

Note : every interval width $M_j - M_i$ can be different

An example of calibration curve is plotted just below

Mass calibration curve (B^2 is given in arbitrary unit)
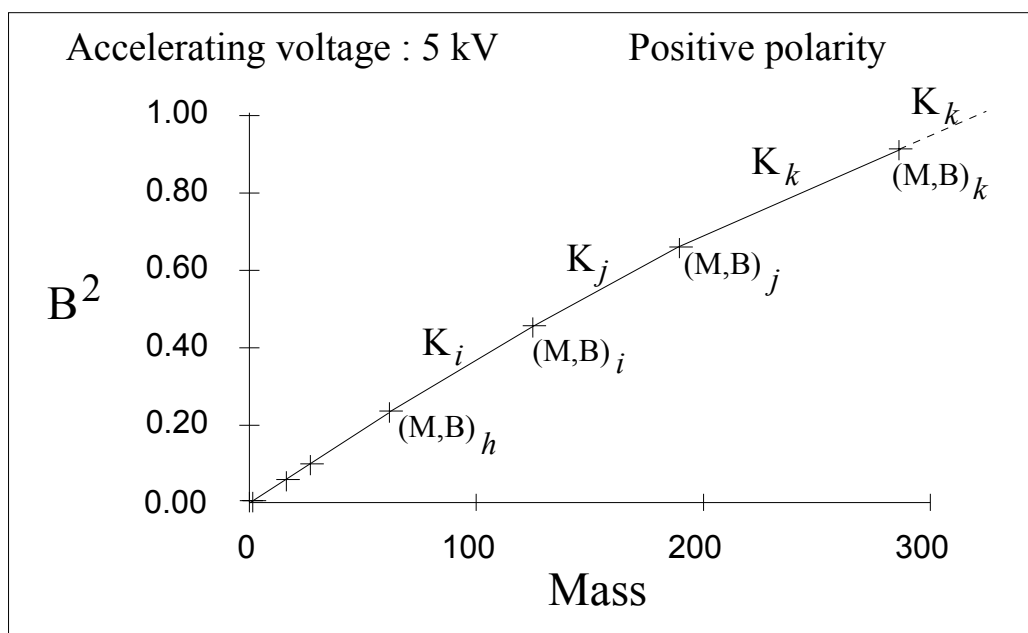
2.1.2 The IMS1270 four mass ranges

The magnetic field B is coded with 19 bits; its maximum numerical value is therefore 524 288. The B numerical value is displayed in the *Tuning* panel if the *B field* option is selected, instead of *Mass*. Four mass ranges can be manually switched on the magnet power supply chassis, located at the back of the instrument, underneath the coupling line. At a secondary voltage of 10KV, these 4 mass ranges correspond respectively to M=300, M=150, M=75 and M=40. In other words, if the range R300 is selected, the maximum value 524 288 corresponds approximatively to the Mass 300 a.m.u, at 10KV, and to the mass 600 a.m.u at 5KV.

The range R300 is the more commonly used. Other mass ranges are selected whenever an analysis requires only low mass measurement at high resolution. For example, let us suppose that the largest mass range, R300, is selected with a secondary voltage of 5KV. The full scale, 524 288 corresponds to M=600, and M=17 will be obtained for B=88250. In this case, an increment of one digit will lead to a relative mass increase of 23 ppm. Such a resolution is not sufficient to center a flat top peak at a mass resolution of 6000 (See the IMS1270 ion optics user's guide). The operator must then switch to a lower mass range, according to the higher mass to be analysed.

A given *[M, B]* table is suited for a given configuration (Mass range, Sec Voltage) Whenever the user either switches the mass range or modifies the Sample HV, he must load the corresponding *[M, B]* table.

The following table gives the relationship between the hardware Mass Range, the sample HV and the measurement displayed on the Hall probe Voltmeter (located on the measurement chassis front panel).

	Sample HV=10KV	Sample HV=9KV	Sample HV=5KV
Mass Range R1	$M = 300$ $V_{hall} = 10$	$M = 333$ $V_{hall} = 9$	$M = 600$ $V_{hall} = 5$
Mass Range R2	$M = 150$ $V_{hall} = 5$	$M = 167$ $V_{hall} = 4.5$	$M = 300$ $V_{hall} = 2.5$
Mass Range R3	$M = 75$ $V_{hall} = 2.5$	$M = 83$ $V_{hall} = 2.25$	$M = 150$ $V_{hall} = 1.25$
Mass Range R4	$M = 40$ $V_{hall} = 1.33$	$M = 44$ $V_{hall} = 1.20$	$M = 80$ $V_{hall} = 0.67$

2.1.3 Computing the magnetic field B after the table *[M,B]*

In different programs, for example, *Tuning*, *Mass Calibration*, CIPS is requested to compute the magnetic field B from the current [M, B] table. The B computing is achieved as follows:

Let M_k the highest mass calibrated in the mass table. B_X corresponding to the the mass M_X is computed following the relationship :

$$\text{if } M_X \in [M_i , M_j] \qquad\qquad B_X{}^2 = K_j (M_X - M_i) + B_i{}^2 \qquad\qquad (3)$$

$$\text{if } M_X > M_k \qquad\qquad B_X{}^2 = K_k (M_X - M_k) + B_k{}^2 \qquad\qquad (4)$$

2.2 Building-up and modifying a [M, B] table

2.2.1 Overview

Initialization

When clicking *INIT*, the [M, B] table is initialized with the point (0, 0) and the point (M_{range}, B_{max}), where M_{range} is the mass which was edited in the editing field *Range* of the main *Mass Calibration* panel .

Adding a new point to the current table

A new point is added into the table by calling the *MASS CALIBRATION* program from the *TUNING*. 2 cases are to be considered:

- Clicking *DIRECT CALIB* from the *TUNING*. Then, the current point (M, B) is added to the [M, B] table without opening *Mass Calibration* program windows.
- Clicking *CALL CALIB* from the *TUNING*. Then, the point will be added after the operator clicks VALID in the Mass Calibration Panel.

Removing a point from the current table

This can be achieved by displaying the [M, B] table with *DISPLAY CALIB* and to use the *Delete* function.

Modifying the overall current table

The overall table can be shifted by using the program *SHIFT CALIB* function.

Save/Load

Adding or deleting a point modifies only the current table. These modifications will be saved only if the operator uses the function *SAVE*. It will be then possible to recall further the saved table with the *LOAD* function.

The overall Mass Calibration program is presented in the section § *Defining and Running an Isotope Analysis*, subsection § *Calibrating the magnetic field before the analysis.*

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2.2.2 The Main *MASS CALIBRATION* Panel

SAMPLE HV, `DISPLAY Field`, is the sample HV which was recorded in the current [M, B] table file when it was created.

POLARITY, `DISPLAY Field`, is the sample HV polarity which was recorded in the current [M, B] table file when it was created.

MASS RANGE, `DISPLAY Field`, is the Mass Range, recorded in the current *[M, B]* table file and corresponding to 524288 digits.

Mass and ***Bfield***, `DISPLAY Fields`, display the current Mass and Bfield.

MRP, `EDIT/DISPLAY Field`, is initialized as the Analysis Mass Resolution *MR* if the mass calibration routine is called from Analysis or the last used value if it is called from *Tuning*. It can be also be edited by the operator and will then determine the scan width (See the hereunder section § *Calibrating the magnetic field before the analysis*) .

Set calib detector (EM/FC1/FC2/L'2/L2...)   selects the detector involved in the *Mass Calibration*.

CYCLING *(TAGGED/NOT TAGGED)* selection: If *CYCLING* is tagged in blue, that means that the B field is always controlled under the current analysis cycle, with the actual analysis timing. No calibration can be achieved in this mode.

DISPLAY CALIB   allows to display the current [M, B] table and to delete one or several point if required. See the hereunder section § *Modifying a [M, B] table from DISPLAY CALIB.*

SHIFT CALIB   allows to shift the overall [M, B] table. See the hereunder section § *Modifying a [B, M] table from SHIFT CALIB*

CALIB TOF   allows to display and to build the table [M, TOF]. See the hereunder section § *Procedure for Calibration the TOF (Time of Flight)*

MASS CAL. MANUAL allows to perform a manual calibration and opens the corresponding dialog box. See the hereunder section § *Manual Mass Calibration*

MASS CAL.SEMI-AUTO allows to perform a semi-auto calibration and opens the corresponding boxes. See the hereunder section § *Semi-Auto Mass Calibration* .

CENTER TROLLEYS Is used for the multicollector, once a given mass peak has been adjusted with respect to the corresponding detector, it allows to center mechanically the other moving detectors with respect to other ion peaks. See the hereunder section § *The Multicollection Center Trolley Panel* .

CALIB.FROM TABLE/ CALIB FROM CONDITIONS This selection is used only when the *Mass Calib* is called from *Analysis definition*. Whenever *CALIB FROM TABLE* is selected the initial *Bfield* corresponding to each mass is derived from the *[B, M]* table. Whenever *CALIB FROM CONDITIONS* is selected the initial *Bfield* comes from the analysis *[m, b]* table. See the hereunder section *The Mass Calibration [m, b] table*

FILE NAME DISPLAY Field displays the current *[M, B]* table filename.

QUIT closes the Mass calibration window.

File (load/ save/ save as/ Init new file/Init new file /file info allows to load and save a *[M,B]* table. See the next hereunder panel.

Load allows to load a previously stored *[M, B]* table file. The loaded table becomes the current *[M, B]* table. If the Sample HV, the secondary polarity and the Mass Range do not fit the instrument current status, an error message appears.

Save, Save as allows to save the current *[M, B]* table. If the current *[M, B]* table has not yet been saved, it will not be lost in case of a computer crash and will be backed up providing that the operator answers "yes" when the software is restarted.

Init New File is used for initializing a new *[M, B]* table. It activates the reading of *SAMPLE HV*, *SECONDARY POLARITY* and *MASS RANGE*. *MASS RANGE* is not read from the hardware but from the set-up. After the reading, these 3 fields can be edited as well.

File Dialog box
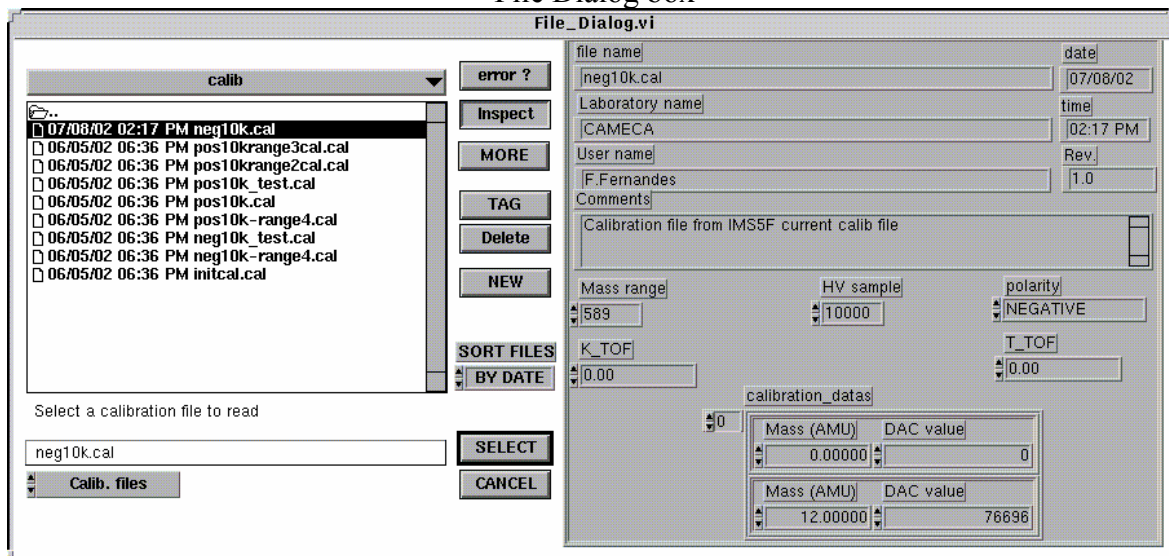
For K_TOF and T_TOF, See the hereunder section § *Procedure for Calibrating the TOF (Time of Flight)*

Calibration_datas are purposed for the *[B, M]* initialization.

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2.2.3 Initializing the current [M, B] table

- Click *File/Init new file* in the main *Mass Calibration* panel. *Sample HV*, *Secondary Polarity*, are then read in the *General Set-up* panel (See the section § *The instrument Set-up panels*) and displayed in the fields located in the main *Mass Calibration* panel.
- If required, edit modifications of the *sample voltage* and of the *range* fields. It is a way for modifying the *General Set-up* panel.
- It is recommended to calibrate (*DIRECT CALIB*, from the *Tuning*) a real mass close to the upper limit of the range, and then to delete the second default point which was created by the table initialization.
- Save the file.

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2.2.4 Modifying the current [B, M] table from *DISPLAY CALIB*

Click *DISPLAY CALIB* in the main *Mass Calibration* panel. The graphic window *DISPLAY CALIBRATION* is then opened.
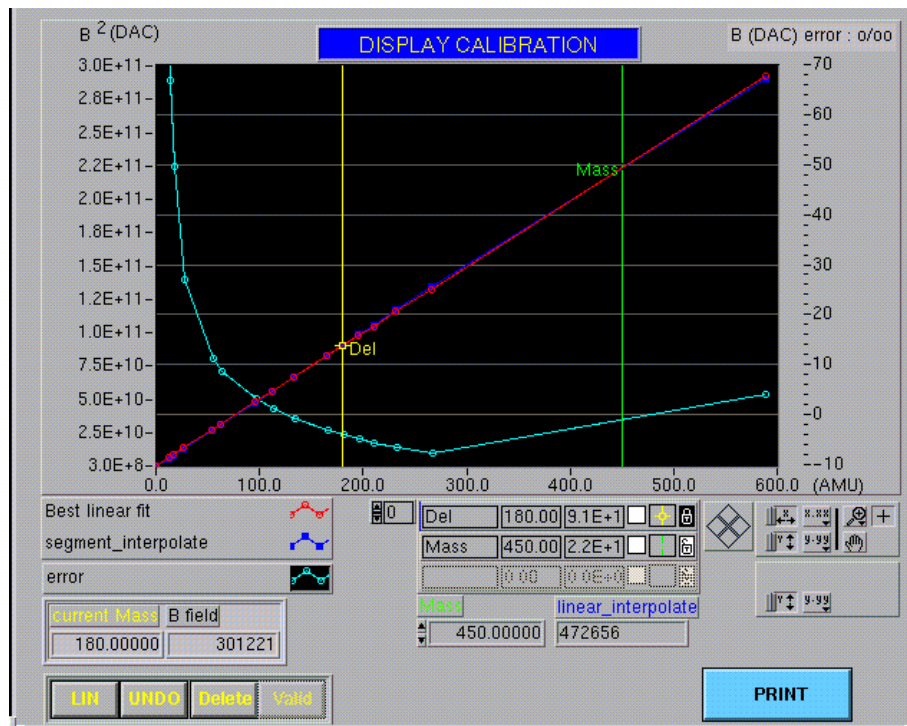
3 curves are displayed in the graphic window. The Y-scale is in B^2, so that the points (M,B) are on a straight line in a first approximation.

- The [M,B] curve, *segment_interpolate*, consisting of the actual table points, and linear interpolation between these points.
- The line Best linear fit, which fits as close as possible the actual curve [M, B]
- The difference between the first 2 curves, error, targetted to point out an spurious point (for such a point, the difference between the 2 curves is expected to be far larger than for the other points.)

2 cursors are available: a yellow cursor *Del* used for deleting a point and a green cursor *Mass* dedicated to the diplay of the exact values in the display fields *current Mass* and *B field*.

LIN/LOG allows to change the scale. Note that there is no reason to use a *LOG* scale
UNDO allows to restore the point which has just been deleted
Delete + VALID allows to delete a point of the [M, B] curve: put the yellow cursor *Del* onto the point to be deleted, and click *Delete*. (The *Del* cursor option must be *Snap to point*)

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2.2.5 Modifying the current [M, B] table from the Mass Calibration program or with Direct Calib

Adding a new point or modifying a previous registered point requires to use the function *DIRECT CALIB* (See the hereunder section § *The main Tuning panel*) or to call the program *Mass Calibration* from the tuning.

DIRECT CALIB is the easiest way for adding a point to the [M, B] table: Set the Mass M in the *Tuning* Panel. Set the B field by using the keyboard Mass thumbwheel (The actual value of B is then displayed in the *Tuning* panel). Then click *DIRECT CALIB*

CALL CALIB can be used as well. It opens the main *Mass Calibration* panel. It is then required to use the *Mass Calibration* program. See the sections § *The Manual MASS CALIBRATION panels* and § *The Semi-Auto MASS CALIBRATION panels*. A (M, B) point is added or modified in the current [M, B] table when clicking *ALL DONE*.

When using the *Mass Calibration* program from *Analysis Def* or from *Analysis*, the calibrated values of B are directly included in the current analysis mass table, but not registered in the [M, B] table.

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2.2.6 Modifying a [B, M] table from *SHIFT CALIB*

The *SHIFT CALIB* function allows to transform the current [M, B] table according to the relationship

$$B_i(new) = B_i(old) \; x \; B_{ref}(new) \, / \, B_{ref}(old)$$

Where $B_{ref}(new)$ is the current B field value and $B_{ref}(old)$ is the value of B corresponding in the previous [M, B] table to the current Mass, as it is displayed in *Tuning*.

Procedure
- In the *Tuning* Panel, set the mass which will be used as reference and set the B field with the keyboard thumbwheel.
- Click *CALL CALIB*.
- In the main Mass Calibration Panel, click *SHIFT CALIB*.
- A small box is then opened in the *Mass Calibration* panel, allowing to select the mass range the shift operation will be applied on. In this small box, if *OVER RANGE* is selected, the shift will be applied for the overall table. If *IN THE RANGE* is selected, the shift transformation will be applied only between *Low Mass* and *High Mass*, contained in the small box editing fields.
- In the graphical window, click *DO+VALID*.
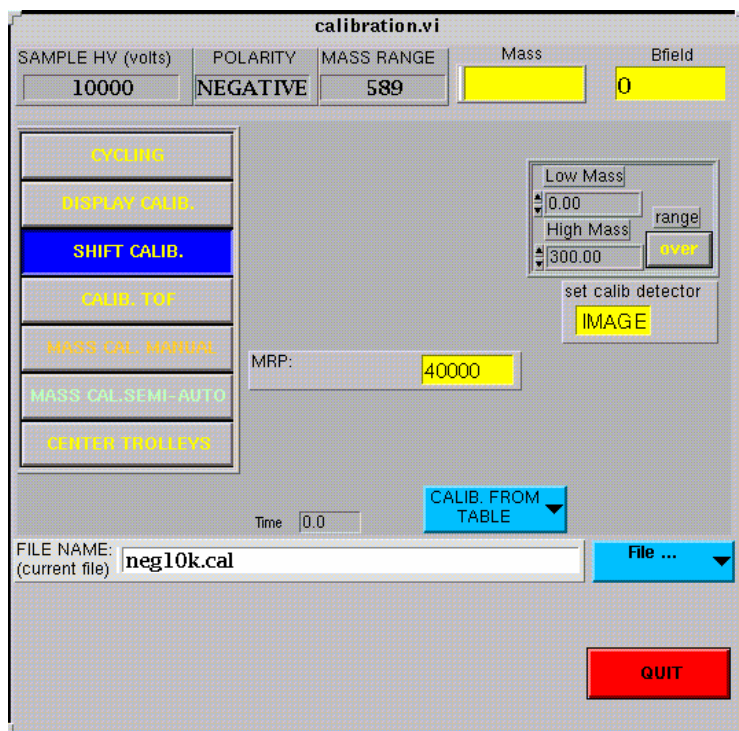
The *SHIFT CALIB* Panel

The graphical window which is opened when clicking *SHIFT CALIB* is identical to *the DISPLAY CALIB* graphical window, except that Delete is replaced by *DO*. *UNDO* cancels the last *DO* action.

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2.2.7 Procedure for Calibrating the TOF (Time of Flight)

As the velocity of ions is not infinite, there is a delay between the primary beam rastering and the ion detection which must be taken into account to reconstruct scanning ion images. This delay, called *Time of Flight* (TOF), depends mainly on the secondary ion mass and on the secondary voltage:

$$TOF(\mu s) = 2.285 * L(m) * \sqrt{\frac{M(amu)}{U(KV)}}$$

L, the distance between the sample plane and the EM, is 6.3m for the IMS1270. This gives 72 µs at 10KV for the mass 250. This is not negligible for the scanning ion image, since the pixel time is 2µs at the lower scanning rate and 0.2 µs at the higher scanning rate.

For a given mass, the TOF is determined by tuning the SII image (See *The IMS 6F/ IMS 1270 User's guide,* section § 6.2 *Scanning Ion Image*). The TOF calibration makes it possible to record several points (M, TOF), to deduce the pair of coefficient K_TOF and T_TOF of the best fitted function

$$TOF = T\_TOF + K\_TOF * M^{1/2}$$

Normally, only 2 points are necessary for determining the pair of coefficients, but more than 2 points can be recorded and taken into account. The TOF calibration parameters are saved in and loaded from the same file than the mass calibration table.

Procedure
- On the main Mass Calibration panel, click
- Select the required mass on the *Tuning* panel, tune B with the keyboard mass thumbwheel. An EM signal is obtained.
- Adjust the TOF correction value on the SII chassis.
- On the graphical TOF CALIBRATION panel, click ADD + VALID. The TOF calibration curve is updated (the curve is plotted only after the second point of the curve has been calibrated).

The TOF CALIBRATION panel
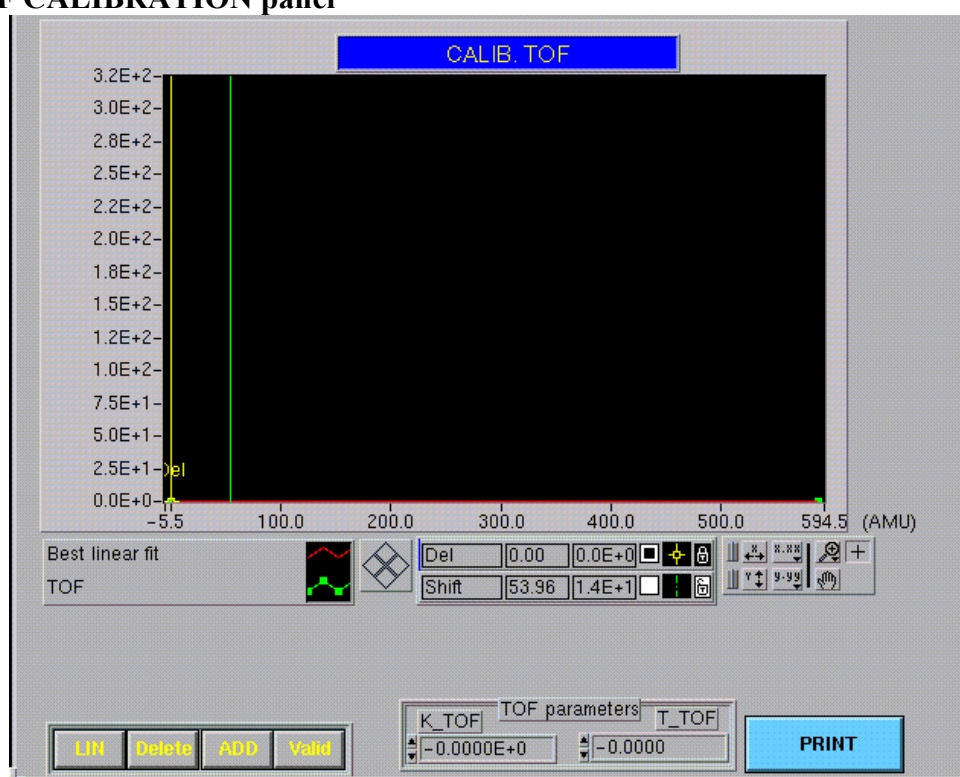
ADD for adding a new point
Delete for deleting a point
VALID must be made before leaving the application for taking into account the modifications in the current [M, B] table

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2.3 The [M, B] table files and the SAVE and LOAD functions.

The [M, B] files are normally stored in the sub-directory *calib*

In the main *Mass Calibration panel*, click *File*

Save, save as This function saves, on the hard disk, the current [M, B] table. A box is opened. Type a file name in the *file name* field. This box can be used as a [M, B] file manager. The parameters displayed in the main Mass Calibration panel (Secondary Voltage, polarity and mass range) are saved in the [M, B] file and the TOF coefficients as well. It is recommended to give an explicit filename (for example neg_9KV_mass70)

Load The [M, B] table file manager box is opened and allows to load the selected [M, B] table as the instrument current [M, B] table. This loaded table replaces the previous current [M, B] table (do not forget to save it, if required). The secondary voltage, the polarity and the mass range are displayed in the main *Mass Calibration* panel. The TOF coefficients are loaded as well and replace the previous.

Init New File This function erases the current [M, B] table and creates a new table with 2 points (0, 0) and (M_{range}, B_{max}) where M_{range} is the value displayed in Range, and B_{max}=524288

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3. Starting the Instrument

3.1 Saving and restoring Keyboard files

3.1.1 Overview

The configuration of all the instrument parameters which are controlled from the computer and are normally tuned from the dedicated keyboard can be saved on the computer disk and restored further by using the *COLUMNS* panel, available by clicking *COLUMNS* on the main bar menu. The keyboard file is divided into several parts: *Sources*, *Primary*, *Secondary*, *Detection*, *Presets*, *Motors*, which can be saved and loaded independently. The lists of parameters contained in these different files can be read in *The IMS1270 dedicated keyboard user's manual* and in *User's guide for Multicollector* for the multicollector parameters saved and loaded with the *Detection* option.

Practically, when the user wants to change a keyboard file, it is recommended to perform a *Global Download*. Normally this operation occurs whenever the main ion optical parameters (Source, primary voltage, secondary voltage, sample z) must be changed. As long as these main parameters are constant, the same keyboard file can be used and only *Start and Stop Source* operations will be performed.

The partial *save* and *load* operations are recommended for *Detection* concerning the multicollector which may be not used. Partial *save* and *load* operations concerning the *Primary* parameters, the *Secondary* parameters, the *Preset* or the *motor* parameters are useful especially at the first steps of the instrument setting on, for building the main keyboard files.

The keyboard files are normally saved in the .... directory. All the global keyboard files contains one type of sources among Cs+/Ga+/O2+/O-/O2-/Ar+ and they will be sorted depending on this source type.

For more details about the save and restore keyboard file issue, read *The IMS1270 dedicated keyboard user's manual*, § *Appendix7: Saving and Restoring the keyboard files*.

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3.1.2 The *COLUMNS* panel
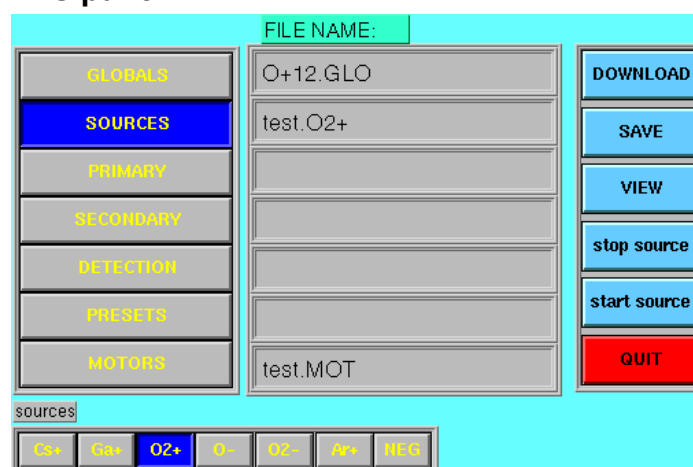
Left hand side bar
GLOBALS/SOURCES/PRIMARY/SECONDARY/DETECTION/PRESETS/MOTORS

Selects which part of file will be *downloaded*, or *saved* or *viewed* (display of parameter values on the computer screen).
Global Download includes also a possible *start source*.

Bottom bar
Cs+/Ga+/O2+/O-/O2-/Ar+/NEG

This bar appears only if the *Source* button is blue. It selects the source which will be *started* or *stopped*.
Cs+ indicates Cesium Source
O2+ and **Ar+** indicates the Duo Source in the positive polarity. The selection *O2+/Ar+* implies only a file sorting.
O2- and **O-** indicates the Duo Source in the negative polarity. The selection *O2-/O-* implies only a file sorting.
NEG indicates the Electron Gun

Right hand side bar

DOWNLOAD Restore a saved file and loads the parameters towards the intrument hardware.

DOWNLOAD + GLOBALS opens the opposite dialog box. The buttons allow to select some options:
Source (Cs+)
• The download process will include *Start Source* only if the source button (*Cs+*) is blue.
Motors
• *MOT* is not blue: Nothing concerning the aperture motors is loaded.
• *MOT* blue: Apertures positions and width are restored.
Multicollector
• *DET* is not blue: The Multicollector parameters are not loaded.
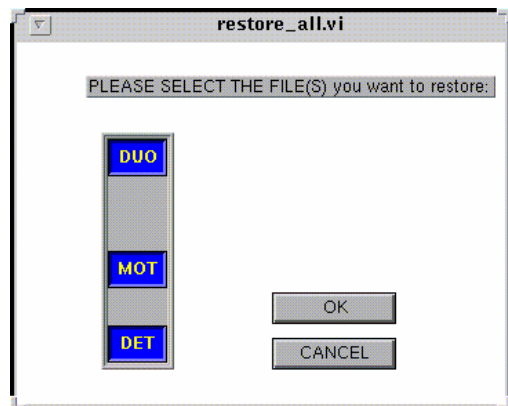
SAVE saves the current keyboard parameters with a filename edited in a dialog box. A first dialog box allows to select the type of source which must be associated with the file.

VIEW allows to read (but not to edit) the parameters contained in any stored keyboard file.

Stop source, **Start source** allows to run the automatic procedure of starting or stopping a source. A dialog box allows to select the type of source and to delay the *Start* or *Stop* operation.

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3.1.3 Starting and stopping the source

A detailed descrition of both Start and Stop source process is given in *The IMS 6F/ IMS 1270 User's guide,* Chapter *Keyboard functions,* section § *Duo source files, Cs source files, NEG source files.*

Clicking Stop Source opens the hereafter panel
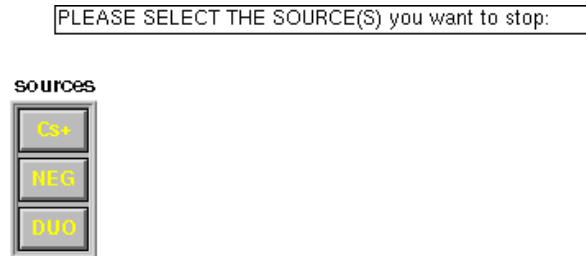
Cs+/NEG/Duo selects the source which must be stopped.

Apply runs the source stop routine.

3.1.4 The source counters
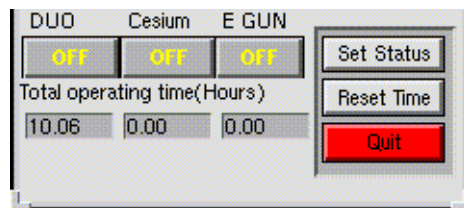
This panels is displayed whenever CIPS is opened. The source status (ON/OFF) are displayed, and for every source the number of ON hours since the last reset.
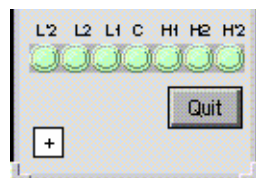
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3.2 The instrument Set-up panels

The set-up panels are targetted to configure the software accordingly to the hardware actually implemented. It is necessary to call and modify the set-up panels whenever the hardware is modified; Most of these modifications are normally achieved by the Cameca Service engineers, but the user may also achieve some modifications by himself, for example:

- Switching the mass range
- Mounting different diameter contrast apertures or new slits onto the multicollector trolleys.
- Changing the multicollector detectors.

For calling the set-up panels, click *Set-up* on the *Tools* bar of the main menu. There is 3 different *Set-up* panels, swichable with the button located at the left bottom corner of each

panel: *General Set-up/ Hardware Set-up/Detection Set-up*. These different panels are displayed and commented in the section § *The Setup panels* in the *user's manual (2)*

On the *general Set-up* panel, *Mass Range (300/150/75/40)* is the hardware switching which can be manually selected at the instrument rear side. It corresponds to different ranges of the Magnet power supply.

<div style="border:1px solid black">

Whenever the operator switches the Mass Range, he must update the set-up panel corresponding field

</div>

Note that both fields *Mass Range* and *Energy* can be modified from this panel, but also from the main Mass Calibration panel (See above the section § *Initializing the current [M, B] table*)

Mass Range "300" means that at 10KV secondary voltage, the on axis mass at the exit magnet will approximatively 300 for the maximum magnetic field maximum value 524 488.

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4. Checking the instrument before an analysis

4.1 Overview

Once the instrument is correctly configured for an analysis (suitable kbd file is loaded, suitable source is started, the [M, B] table corresponding to the secondary HV is loaded), before starting an analysis, the operator must check that the instrument is ready for analysis:

- First the operator must obtain some signal on the MCP device and on the main axis detectors. The Tuning panel will be involved (see the hereunder section § *The main Tuning panel*). The operator will then be able to play with the dedicated keyboard (See the *IMS1270 dedicated keyboard user's manual*)
- Then the operator must check that the instrument is correctly tuned for the planned analysis. (See the *IMS1270 ion optics User's manual*). For this purpose, it will be necessary to estimate the mass resolution by looking at the MCP video camera image, and in order to measure it more accurately, by achieving and featuring a High Resolution Spectrum. (See the hereunder section § *Checking the Mass resolution and the peak flatness*).
- In the case of a multicollection analysis, the operator must also position correctly the moving collectors. (See the hereunder section § *Multicollection case: Setting the trolley positions*).

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4.2 Tuning the instrument

4.2.1 The main *Tuning* panel

Click *Tuning* in the main menu bar
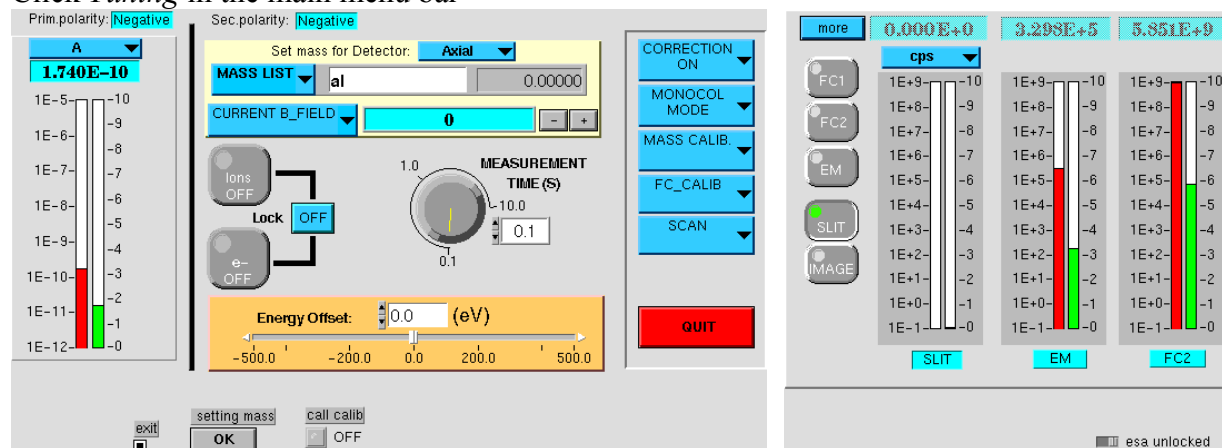
The tuning functions are :

- ➢ Displaying the current primary or secondary intensities in both monocollection and multicollection modes
- ➢ Displaying the current B field value (in digits)

> ➢ Displaying the mass being analyzed according to the B field value read from the magnetic field interface and the mass calibration table.
> ➢ Controlling the magnetic field to change the mass being analyzed.
> ➢ Controlling the sample HV offset.
> ➢ Displaying polarities
> ➢ Activating centering routines useful for aligning correctly and reliably the instrument.

The primary current functions

The **primary current bargraph**, at the left hand side diplays the primary current when the switch BEAM ON/OFF is OFF (i.e. OFF the sample and therefore blanked into the primary Faraday cup.

IONS OFF/ ON   This switch is the image of the *Beam ON/OFF* key implemented on the dedicated keyboard. It switches the primary ions onto the sample (ON) or onto the primary Faraday cup (OFF).

e- OFF/ ON   This switch is the exact image of the *e- ON/OFF* key implemented on the dedicated keyboard (NEG Electron beam ON or OFF)

Lock OFF/ ON   If *Lock ON*, *IONS* and *e-* are switched togeteher ON/OFF. But if *IONS ON/OFF* or *e- ON/OFF* is switched from the keyboard, both functions are not linked.

PRIMARY CURRENT (above the bargraph) diplays the numerical value of the primary current intensity, in Amperes or in cps, according to the selection **A/cps**

The Mass functions

CURRENT B field   DISPLAY Field Displays the value of the magnetic field in digits (between 0 and 524288) or in a.m.u, according to the selection **Mass/B field**

Mass EDITING Field controls the *Mass* which must be selected by the mass spectrometer. The *Mass* can be edited in a.m.u (i.e. *161.1*) or in symbol (i.e. *Cs Si*, or *29Si*). When a simple symbol is edited (i.e. *Si*), the major isotope is selected by the periodic table (See the hereunder section § *The species table in the monocollection mode*). For loading the magnetic field on the instrument, hit *Enter* on the computer keyboard. The B field will be computed according to the current [M, B] table (See above, the section § *The [M,B] table*)

axial/L'2/L2/.../H1 is purposed for shifting the beam from the main axis to a multicollector given detector. It must be used in the following way. This field is first set to *axial*. Let's suppose that the mass is set to ^{28}Si (27.98). The operator targets to shift this ^{28}Si beam onto the detector L'2 the position on which has been correctly initialized with respect to the main axis. (See below, the section § *Multicollection case: Setting the trolley positions*).
- Switch the field from *axial* to *L'2*
- Si is still in the field *set Mass*. Press *Enter*
- The magnetic field is shifted so that the Si Beam is close to the L'2 detector, and the panel displays *axial* and *29.15* (for example) in the field *Mass*.
- Note that "Direct Calib" corresponds always to the axail case.

The secondary functions

Energy Offset `EDITING Field + cursor` allows to edit a sample voltage offset. For the same purpose, it is also possible to play directly with the dedicated keyboard (See *The IMS1270 dedicated keyboard user's manual*, section § *the source pad*)

MEASUREMENT TIME allows to set the integration time for primary or secondary intensities measured in the tuning program. The MEASUREMENT TIME can be edited in the `DISPLAY/EDITING Field` or set with the mouse on the rotating button.

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The right hand side bar menu

CORRECTION ON/OFF/define Corrections When *ON*, the displayed secondary signals are corrected for the EM deadtime and yield, defined in the *Detection Set-up* panel (See the sections § *The EM Physical principles* and § *Detection Set-up* panel in the CIPS user's manual (2)). *Define Correction* is a shortcut for editing directly the correction parameters.
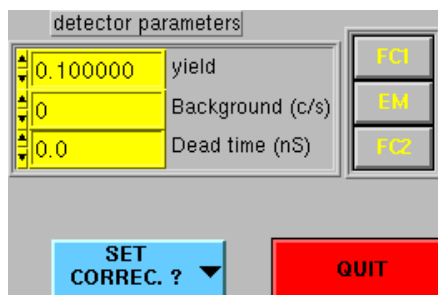
MULTICOL/MONOCOL MODE This selection leads to open the *multicollection Bargraph* panel or the *monocollection Bargraph* panel.

CALIB (DIRECT CALIB/CALL CALIB) allows to call the Mass Calibration program (*CALL CALIB*) or to achieve a direct mass calibration (*DIRECT CALIB*). In this last case, the current pair of values (M, B) will be added to the current *[M, B]* table. See the section § *Building-up and modifying a [M, B] table*.

FC_CALIB: OFFSET/ GAIN & OFFSET opens respectively the *FCs OFFSET CALIRATION* panel (See the section § *FCs Offset Calibration* in the CIPS user's manual (2)) or the *FCs CALIBRATION panel* (See the section § *FCs Calibration* in the CIPS user's manual (2)).

SCAN/ Field Aperture Center/ EM HV Adjust , shortcuts for running useful routines. *Scan* allows to scan any parameter and to record any measurement channel ouput (See the hereunder section § *The Scan parameter panel*). *Field Aperture Center* scans and centers the beam with respect to the *Field Aperture* (See the hereunder section § *The Scan parameter panel/ Field Aperture Center*). EM HV Adjust allows to reajust the Electron Multiplier High Voltage all along the EM life (See the section § *EM HV Adjust* in the CIPS user's manual (2)) .

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4.2.2 The *Tuning Bargraph* panel

According to the selection *MULTICOL/MONOCOL*, the Multicollection or the Monocollection *Tuning Bargraph* panel is opened. For information about the *Multicollection Tuning Bargraph* panel, see the hereunder section § *The Multicollection Tuning panel*.
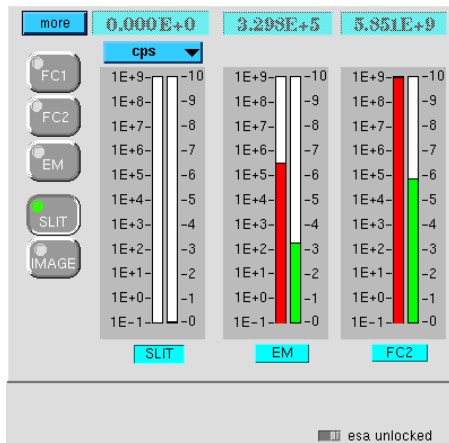
more/ less diplays either simultaneously the 3 *EM-FC1-FC2* bargraphs (*more*) or just a single bargraph (*less*).

EM/FC1/FC2/SLIT/IMAGE allows to switch the secondary beam either to *EM* or to *FC1* or to *FC2* or to the *MCP*, with the *SLIT* mode or with the *IMAGE* mode.

cps/nA allows to display digitally the 3 channel signals in counts per seconf (cps) or in nanoamperes (nA)

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4.2.3 The Scan parameter panel

The function *Scan parameter* allows to select any keyboard parameter and any detector, to scan the parameter in order to record a curve *S(param)*, *S* being the detected signal. It is also possible to compute the center of the curve and to automatically set the parameter to the value corresponding to this center. For more detailed information about the keyboard parameters (their labels, their classification into primary, secondary, detection groups... See *The IMS1270 dedicated keyboard user's manual*.
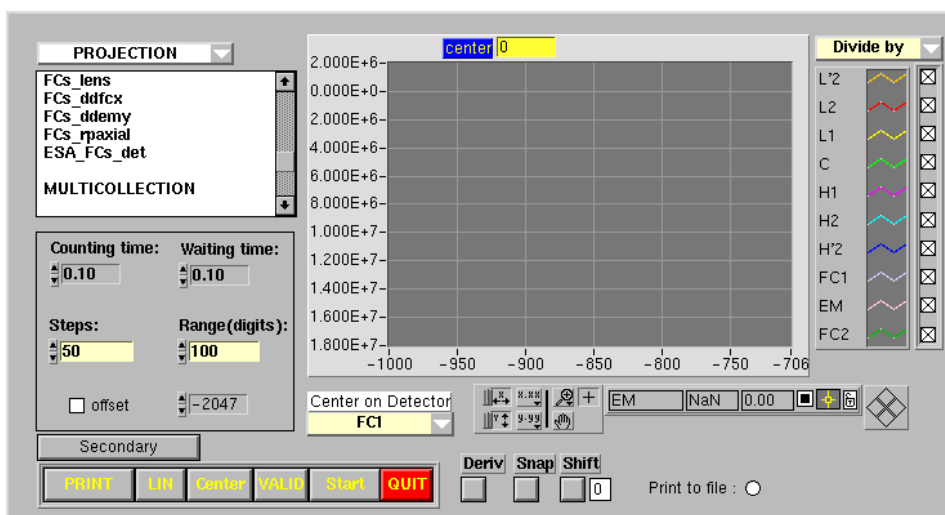
The box located at the left top corner is purposed to the ***parameter selection***

The bar located at the right hand side is purposed to the ***detector selection*** (L'2/L2/L1/C/H1 /H2 /H'2/ FC1/EM/FC2). Several detector can be selected.

Divide by L'2/L2/L1/C/H1 /H2 /H'2/ FC1/EM/FC2 allows to diplay and to process a signal ratio instead of a single signal.

Scanning parameters

counting time EDITING Field counting time per scanned point (typ 0.1 s)

waiting time EDITING Field waiting time before each scanned point (typ 0.1 s)

steps EDITING Field number of scanned points. (typ 50 points)

Range EDITING Field overall range of the scanning, given in digits. (typ, 300 digits for the entrance slit, 1000 digits for Sple HV, 300 digits for DSP2Y)

Offset EDITING Field the parameter will be set to the computed center of the curve + the offset (typ 0, except +20 digits for Sple HV)

The lower bar menu

PRINT for printing the graph

LIN/LOG graph scaling option

Center computes the center of the curve X_{center} (The maximum Y_{max} is firstly computed. X_{left} and X_{right}, corresponding to the interpolated points such as $Y(X_{left})= Y(X_{right})=Y_{max}/2$, and finally, $X_{center} = (X_{left}+X_{right})/2$. If several detectors are selected (for the multicollector tuning), the curve to be computed is selected in the box *Center on detector*, located just under the graphical window.

VALID After a center operation, clicking *VALID* actually sets the parameter center value.

START/RUNNING Clicking *START* launches the scan. At the end of each scan, the displayed curves are erased and another scan restarts automatically as long as the user does not click *RUNNING* for stopping the scan

Deriv if this button is marked, the derivative will be displayed.

snap Q24 if this button is marked, several scans corresponding to different detector selections can be displayed in the same graph, providing the same parameter is scanned.

shift If this button is marked, it is possible to display on the same graph several scan, corresponding to different parameters, providing the same detector is selected. After clicking shift, the next scan will be saved and displayed. At each shift, the small DISPLAY box at the right hand side of shift is incremented.

print to file It is possible to save the scan function results in a file. Set *print to file* to ON

The *Field aperture Center* case.

When selecting *Field aperture Center* in the *Tuning* panel, 2 full *scan & center* routines will be achieved over the parameters purposed to centre the beam within the *Field Aperture*, *LT1 defatx* and *LT1 defaty*.

The operator is just required to select the detector channel before the routine is started.

Both initial *LT1 defatx* and *LT1 defaty* are displayed in the field x&y.

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4.3 Checking the Mass resolution and the peak flatness

4.3.1 Defining and performing a High Resolution spectrum

As it was pointed out above (See the section § *The main Tuning panel*) a mass spectrum around the current mass can be launched and displayed directly from the main *Tuning* panel by clicking *SCAN* (at the panel right hand side). The displayed spectrum can be printed, but it cannot be processed.

For being able to process a spectrum and thus to feature a peak (mass resolution, flatness), it is necessary to launch a *High Resolution Spectrum*.

The process for running a *High Resolution Spectrum* is very similar to the Isotope analysis (See below the section § *Defining and Running an isotope analysis*)

1. Editing and saving a *High Resolution Spectrum* definition file
From the main menu bar, click *analysis definition* for opening the *ANALYSIS DEFINITION* box.
In the *ANALYSIS DEFINITION* box
- Select *HIGH RESOLUTION* as *Acquisition Mode*
- in *File...*, select *Load* or *New* for opening the *High Resolution Spectrum* dialog box.
- Enter the analysis input data (mass, scan parameters...) in the dialog box.
- Select on *File... /save* or *save as* for saving the analysis definition file.

2. For running a *High Resolution Spectrum*
In the *ANALYSIS DEFINITION* box
- Select the required analysis file
- It is possible to launch the *Mass Calibration* by clicking *CALIBRATE*, though it is generally not required before a High resolution spectrum.
- After the mass calibration (quit the box calibration), click *APPLY* for opening the *ANALYSIS CONTROL* box.

In the *ANALYSIS CONTROL* box
- Click *START*
- The *High Resolution Spectrum* will then be displayed at real time in the analysis graphic window (See below the section § *Defining and Running an isotope analysis*)

> In the *High Resolution Spectrum* scanning process, the B
> field step is always 1 digit.

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4.3.2 Featuring a High Resolution Mass Spectrum with the "Peak Processing"

The curve browser box (See the section § *The curve browser box* in the *CIPS user's manual (2)*) allows to process either the current acquisition, or a previously saved *High Resolution* file.

During the *High Resolution Spectrum* run, the spectrum will be plotted in the *curve graphic window* (See the section § *Displaying and processing the analysis results with the curve panel* in the CIPS user's manual (2))

For processing a *High Resolution Spectrum* peak, click *MEASURE* in the the *curve graphic window.*

A *High Resolution Spectrum* curve can also be processed by the functions available by clicking PROCESS (See the section § *The curve processing functions* in the CIPS user's manual (2)).

The peak information panel
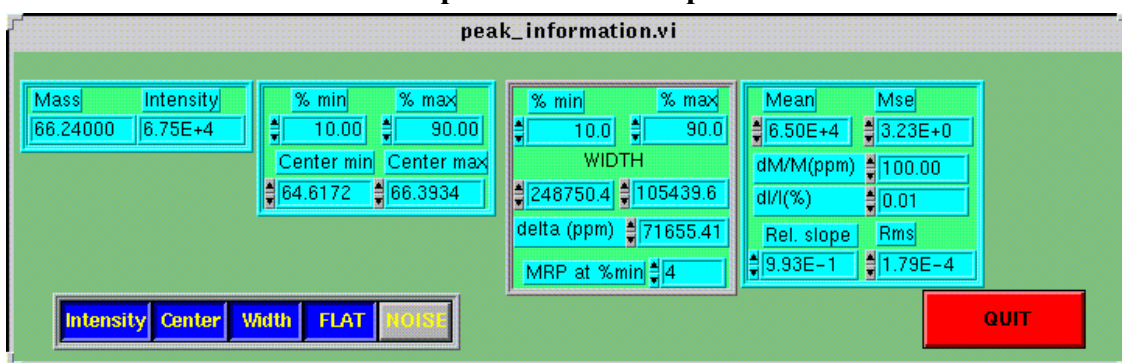
Each button of the panel bottom assigns cursors to special functions and opens a box which displays the peak features. When using any processing function, it is recommended to check that the cursors required for the processing are displayed on the screen. If they are not, check that the cursor color is not transparent. Normally, the useful cursors can be driven with the mouse. This feature is set in the *Graph Properties* panel. It is always possible to move a cursor by blackening the square in the cursor table and by clicking the special cursor button

◈

All the functions are purposed to feature a single peak. It is thus recommended to set the graph scale in order to plot a single peak in the graphic window

Intensity

When clicking *Intensity*, the vertical cursor *#0* is automatically positionned at the curve maximum. It is possible to move the cursor to explore the curve. The *(Mass, Intensity)* box, opened at the *peak_information* panel left hand side displays the coordinates of the curve current point.

Center

The second left hand side (*Center min, Center max*) box is opened. 2 horizontal cursors *#1* and *#2* are assigned to define 2 different levels. These levels (default value: 10% and 90% of the maximum) can be tuned by editing the fields *%min* and *%max* or by moving the cursors manually.

Each cursor   peak intersection defines 2 points. The abcsissa of   center of these 2 points is displayed in the field *Center min* or *Center max*, according to the considered cursor
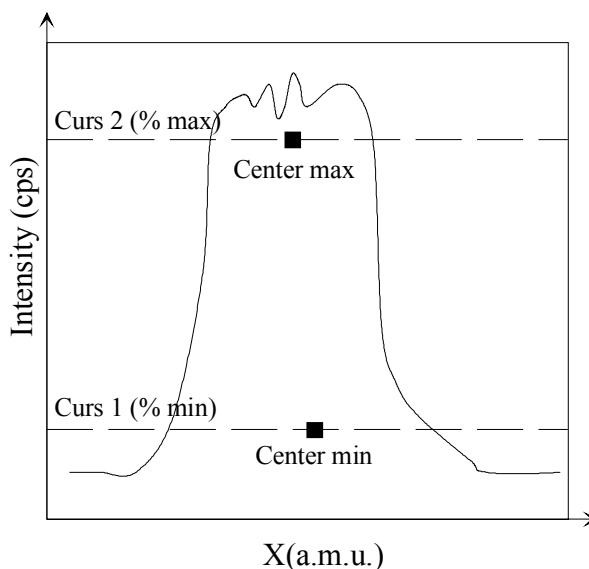
Width

A third box is opened. The horizontal cursors #5 and #6 are used for defining 2 levels editable in the fields *%min* and *%max.*

The 2 display fields located below *WIDTH* contains the respective peak width *Wmin* and *Wmax* corresponding to the respective cursors min and max. *Wmin* and *Wmax* are expressed in *ppm.*

The *delta (ppm)* display field is intended to feature the peak edge width:

$$delta= (Wmin+Wmax)/2$$

The Mass Resolution MRP (display field) is related to *Wmin*

$$MRP= 1\ 000\ 000/Wmin$$
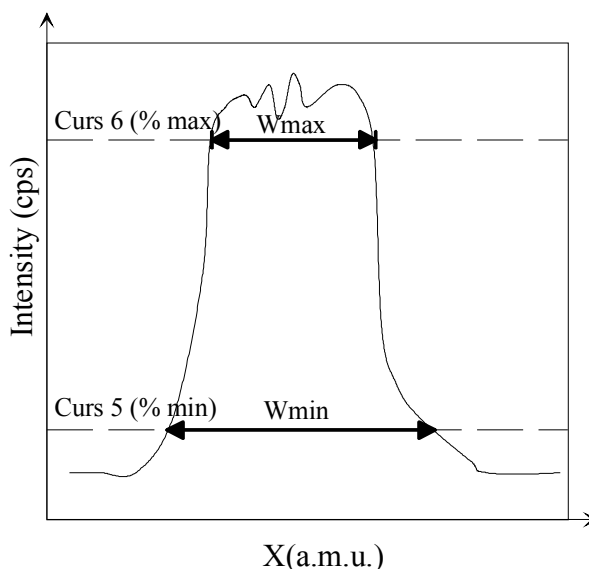
FLAT

The last box, at the right hand side is opened. Vertical Cursors #7 #8 #9 are assigned to this peak flat top featuring. Cursor #8 is the center of both cursors #7 and #9. It is firstly positionned at the curve maximum.

FLAT is dedicated to feature the part of the peak top located between the cursors #7 and #9

The distance between both cursors #7 and #9 is the value displayed in the *dM/M (ppm)* field. This field can be edited. The cursors can also be moved manually.

Mean (display field) is the mean intensity of the peak top.

Mse (display field) is the noise in the peak top interval.

The flat top is approximated by a straight segment which is displayed in the graph.

dI/I (%)(display field) is the difference of intensities between the 2 ends of this segment.

Relative slope is the slope of this segment

Rms is the noise around this segment.

For a more detailed presentation, see below.
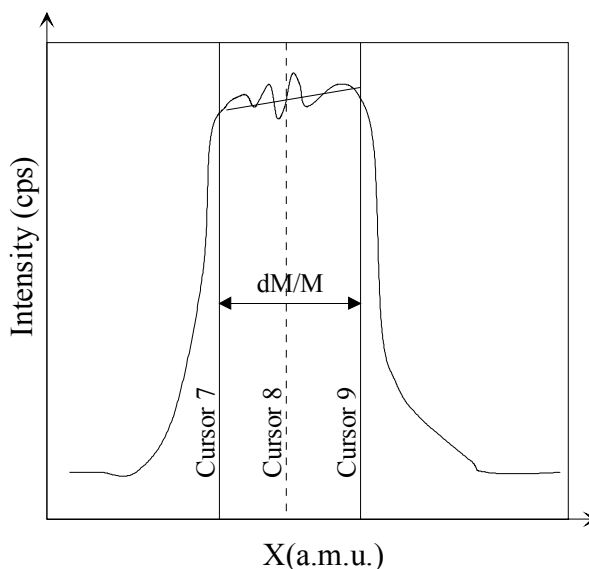
Detailed calculations of the the peak top features

N points are selected between the two cursors. Each point is considered as a pair of coordinates (M_i, I_i) where M_i is the mass number of the measured point i and I_i the recorded signal.

Mean	$Mean \ = \ \bar{I} \ = \ \sum_{i=1}^{i=N} \dfrac{I_i}{N}$

$$\overline{M} \ = \ \sum_{i=1}^{i=N} \frac{M_i}{N}$$

Mse	$Mse = \sigma = \left(\sum_{i=1}^{i=N} \dfrac{(I_i - \bar{I})^2}{N} \right)^{\frac{1}{2}}$
dM/M (ppm)	$dM / M(ppm) \ = \ 10^6 \ \dfrac{M_N - M_1}{\overline{M}}$

Reduced coordinates (m_i, s_i)

$$m_i \ = \ \frac{M_i - \overline{M}}{\overline{M}}$$

$$s_i \ = \ \frac{I_i}{\bar{I}}$$

A **regression linear function** is calculated for fitting the N peak top points

$$s \; = \; \alpha \; m \; + \; \beta$$

dI/I(%)	dI/I = 100 $\alpha(m_N - m_1)$
Relative slope	Relative slope = α
Rms	$Rms = \dfrac{\sigma'}{\bar{I}} = \dfrac{1}{\bar{I}} \left(\displaystyle\sum_{i=1}^{i=N} \dfrac{((I_i - s_i)\bar{I} - \bar{I})^2}{N} \right)^{\frac{1}{2}}$

It is actually considered that the spread among the intensities I_i is generated by two phenomenas:

- A linear drift.

- A stochastic effect.

dI/I and the "Relative Slope" correspond to the linear drift while Rms is the standard deviation once corrected from the linear drift.

NOISE displays 2 parallels segments parallels to the flat top approximated segment, corresponding to the noise level and distant of 1σ from the flat top segment.

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4.4 Multicollection case: Setting the trolley positions

4.4.1 Introduction: The distance/mass multicollector metrology

The multicollector metrology is initialized by clicking *INIT ALL*, in the Multicollection Control box (See below, the section § *The Multicollection Control dialog box*). For locating all the detector positions along the trolley axis, in the same coordinate system, the following data are taken into account:

- 10 mm is the distance between the collector C *end stop* and the main axis.
- The number of motor step between a given moving collector and its *parking stop*.
- A Trolley thickness of 5.5 mm, which actually gives the distance between 2 collector parking stop.
- The *Gap* between the additionnal detectors L'2 and H'2 and their respective main detector L2 and H2

All these data are coded in the software, except the *Gap* which must be entered in the *Detection Set-Up* panel. (See the section § *Detection Set-up* in the *CIPS user's manual (2)*). The *Gap* must be close to 30000. It is equal to the width along the X axis between L2 and L'2 (or between H2 and H'2), in millimeters, multiplied by 2700. The measured width is recorded in the *Multicollector test Sheet* (§1.4, *Collector thickness*: 1-1' and 5-5' are respectively the L2-L'2 and the H2-H'2 width)

The *main axis* is the zero of this *global coordinate system*.

Some of these data have an uncertainty of a few tenth of millimeters, so that, it can be estimated that the displayed position in the Multicollection Tuning panel have a precision of ±2.5mm along the trolley axis, corresponding approximatively to dM/M=±1/1200

> *Multicollector Metrology* precision:
> Trolley axis: ±2.5mm
> corresponding Mass Resolution: 600

In the *Multicollection Tuning* panel, the displayed values of the detector positions are according to coded hereunder relationship between Mass and detector position :

$$\Delta X = 1215 * \frac{\Delta M}{M} + 1600 * \left(\frac{\Delta M}{M} \right)^2$$

$$\Delta Z_{trolley} = 2.7 \, \Delta X$$

4.4.2 The Multicollection Tuning panel

Select Multicol in the main *Tuning* panel (See the section § *The main Tuning panel*)
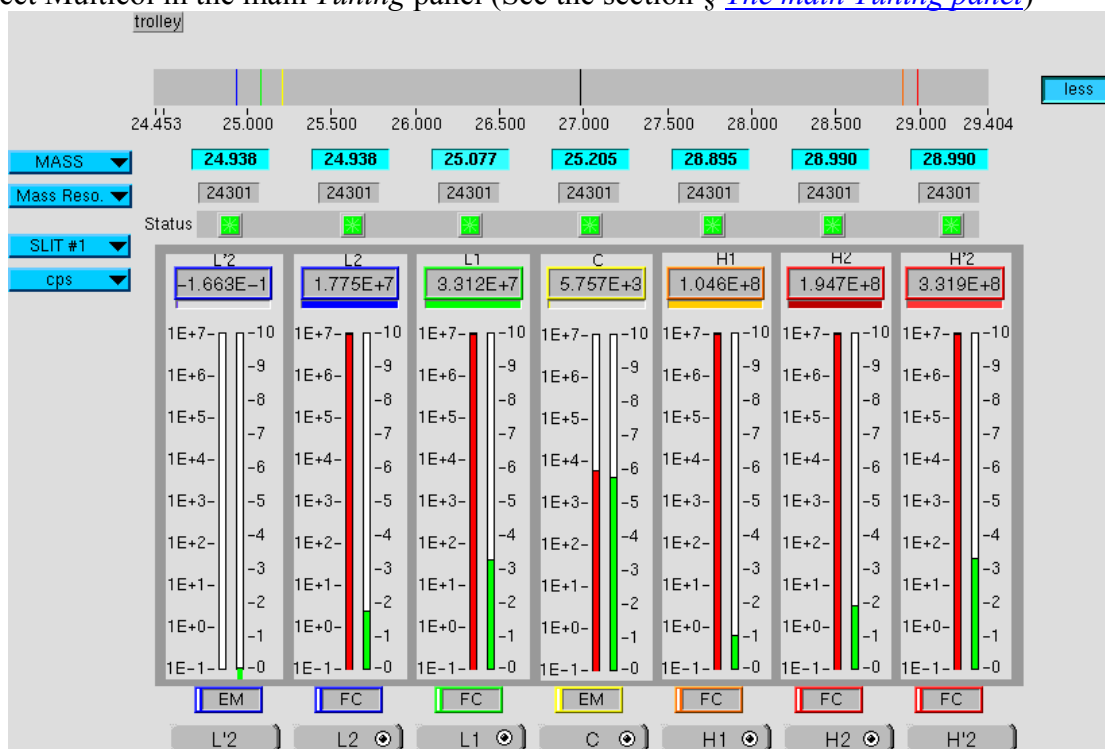
The trolley position display bar This grey bar, at the top of the window displays the location of all the detectors. One cursor corresponds to each collector: Blue for L'2-L2, green for L1, yellow for C, orange for H1 and red for H2-H'2. The black cursor corresponds to the main axis.

MASS/POSITION If *POSITION*, the display field above each detector gives in μm the detector position along the trolley travel axis. If *MASS*, the display field gives expressed in a.m.u. and mean the computed mass corresponding to each detector.

MASS RESO./SLIT SIZE If *SLIT SIZE* is selected, label of the collector entrance slit, as it was entered in the *General set-up* panel (See the section § *General Set-up* in the CIPS user's manual (2)). Each slit number is labelled by a value W_{slit} in microns. If *MASS RESO.* is selected, the Mass Resolution, computed as *$1215000/W_{slit}$*.

Slit #1 /#2/ #3 switches the multicollector exit slits (Standard values are 500μm, 250μm and 150μm)

WARNING: For the same slit position (1/2/3), all the detector slits will be identically labelled, even if different slit bars are mounted onto the different detectors, and the displayed corresponding mass resolution will be therefore identical.

CPS/A DISPLAY Field displays for each detector the measured signal, in cps or in A

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4.4.3 The Multicollection Control dialog box

Open this panel from the main menu *Tools bar* .
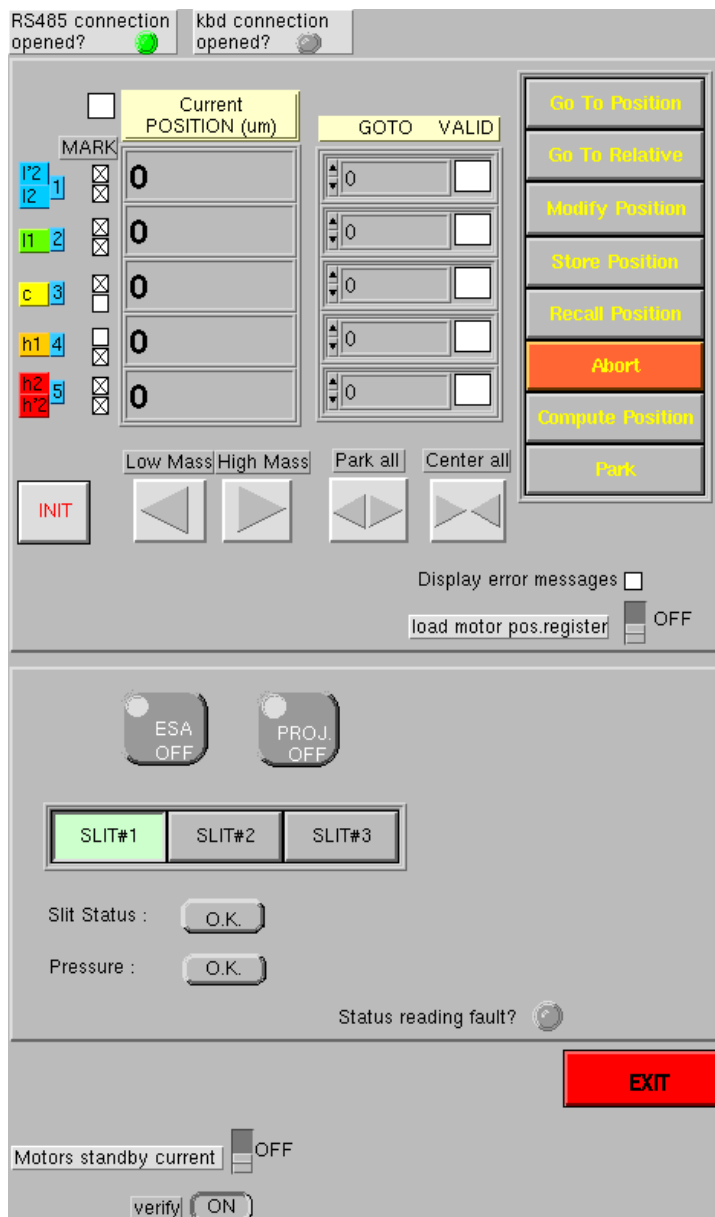
This panel is dedicated to the movable collectors control

Init will measure the total travel of all the trolleys.

MARK The checkboxes, at the left hand side **display** the proximity with other collectors (each movable collector is equipped with an electrical proximity stop.)

CURRENT POSITION (μm) `DISPLAY Field` The trolley position is expressed with respect to its own origin.

Each trolley origin is its parking position.

All the absolute positions are positive.

The position in the Multicollector metrology is displayed only in the *Multicollection Tuning panel* and not in this *Multicollection Control* dialog box,

(GO TO) ***VALID*** Checkboxes are purposed for selecting the collectors which will be actually moved when Clicking *Go to Position* or *Go to relative* . The ***GO TO*** editing fields close to the checkboxes corresponds to the position if it is planned to click *Go to Position* or just to the distance to be run if it is planned to click to *Go to relative* .

Go to Position, Go to Relative

Activates the motion corresponding to the position or the distance which must be edited previously (in μm) in the column "*GOTO*". When pressing "*Go to position*" or "*Go to relative*", only the "*VALID*" channels will be moved.

Low Mass, ***High Mass***

Useful for setting the correct sign of "*relative position*" in the fields *GO TO* .

Store Position, Recall Position

These 3 commands open a dialog box which allows to store, modify and restore a set of collector positions. See this *Multicollector position library* box further in this section.

Modify position Q11

Compute Position opens a panel purposed for helping the user to edit the correct collector position for a given application. See the hereunder Section § *The Multicollection Control Compute box*

Park all will sent the outer trolleys (#1 and #5) at the outer buting parking. The buting parking of other trolleys are the proximity butings between neighbour trolleys.

Center all send all the trolleys close to the axis

INIT Each collector will be driven from its parking location to its end stop, near the main axis, and back to the parking location. This procedure allows to record the total travel of each trolley and to measure each collector in the same global *multicollector coordinate system*. The collector positions in this coordinate system are displayed in the *Multicollector Tuning* panel. (Note that this routine lasts more than 30 minutes)

Multicollector position library

This single table contains all the saved configuration.

A collector configuration corresponds to a line.

Select a line for modifying, deleting or loading a configuration

detectors_list.vi

item	trolley 1	trolley 2	trolley 3	trolley 4	trolley 5	comments
1	9000	9000	9000	9000	9000	

Delete
Clear All
OK
CANCEL
LOAD
SAVE
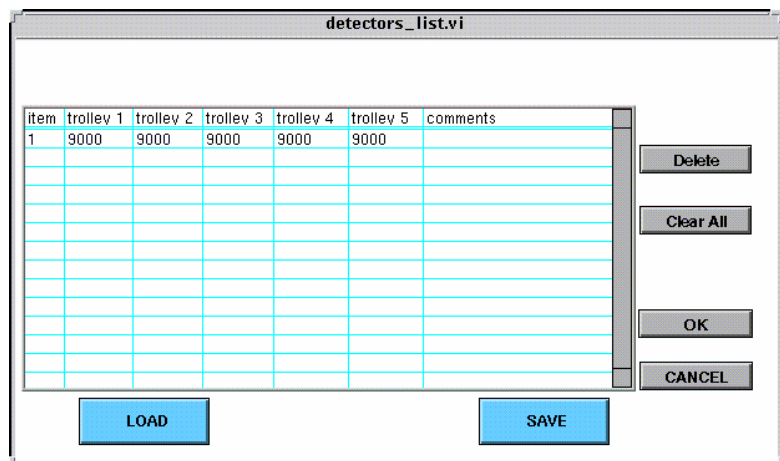
Contents ↑

4.4.4 The Multicollection Control Compute box

Path: Menu Tool bar /Multicol /Compute position button
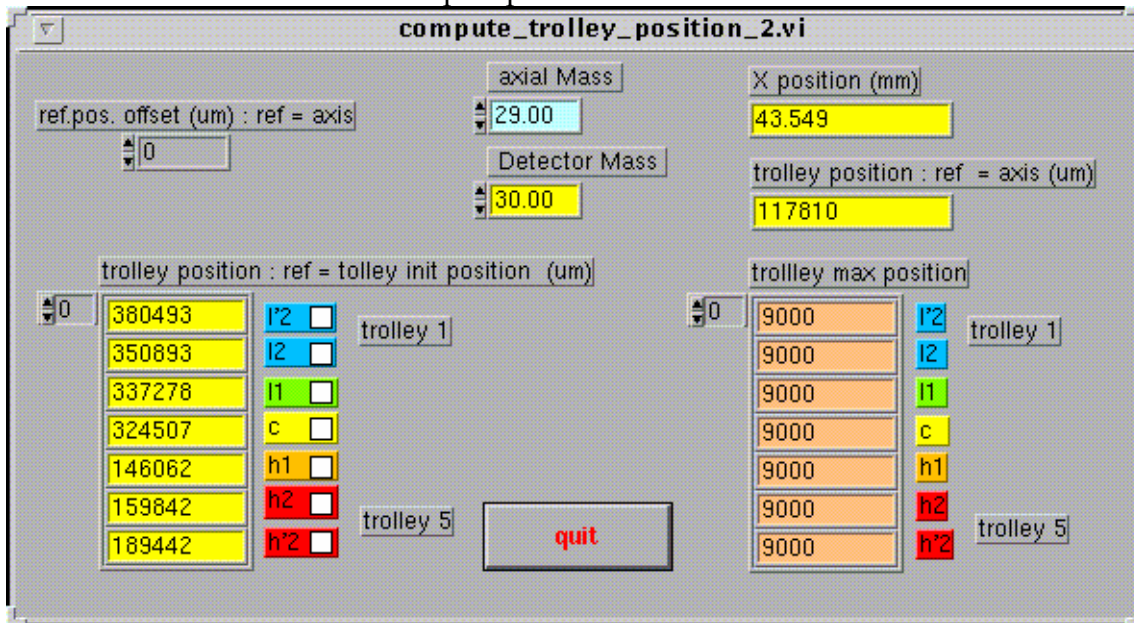
     This tool is purposed for finding the collector positions for a given application. The operator edits in *axial Mass* the mass which is assumed to be on axis. Then, he must edit in *Detector Mass* the mass to be analysed. Once he has decided which collector will be used for this mass, he may transfer the collector position to the main *Muticollection control box* by hitting the checkbox-like close to the considered detector.

ref.pos. offset (µm): ref = axis EDITING Field
Not to be used. To be set to zero.

trolley position: ref=trolley init position (µm) DISPLAY Field
For each detector, the trolley axis position of the *detector Mass*, in its own *detector coordinate system.*

Checkbox-like close to the collector must be used to transfer the collector postion to the main *Muticol. ctrl box GOTO* table

Axial Mass EDITING Field The mass (in a.m.u.) assumed to be on the main axis

Detector Mass EDITING Field The mass (in a.m.u.) to be measured with the multicollector.

X position (mm) DISPLAY Field The X axis position of the *detector Mass*, in the Multicollector *global coordinate system.*

trolley position: ref=axis (µm) DISPLAY Field The trolley axis position of the *detector Mass*, in the Multicollector *global coordinate system.* For the relationship between *X position* and *trolley position*, see above the section § *The distance/mass multicollector metrology*

Trolley max position: DISPLAY Field For each detector, its max position (close to the main axis, 0 being the parking position..

Contents ↑

4.4.5 The Multicollection Center Trolley panel

This panel is targetted to adjust finely the collector positions, after a coarse positionning with the *Multicollection control* and *Compute position* panels. It can be opened from the *Main Mass Calibration panel* .
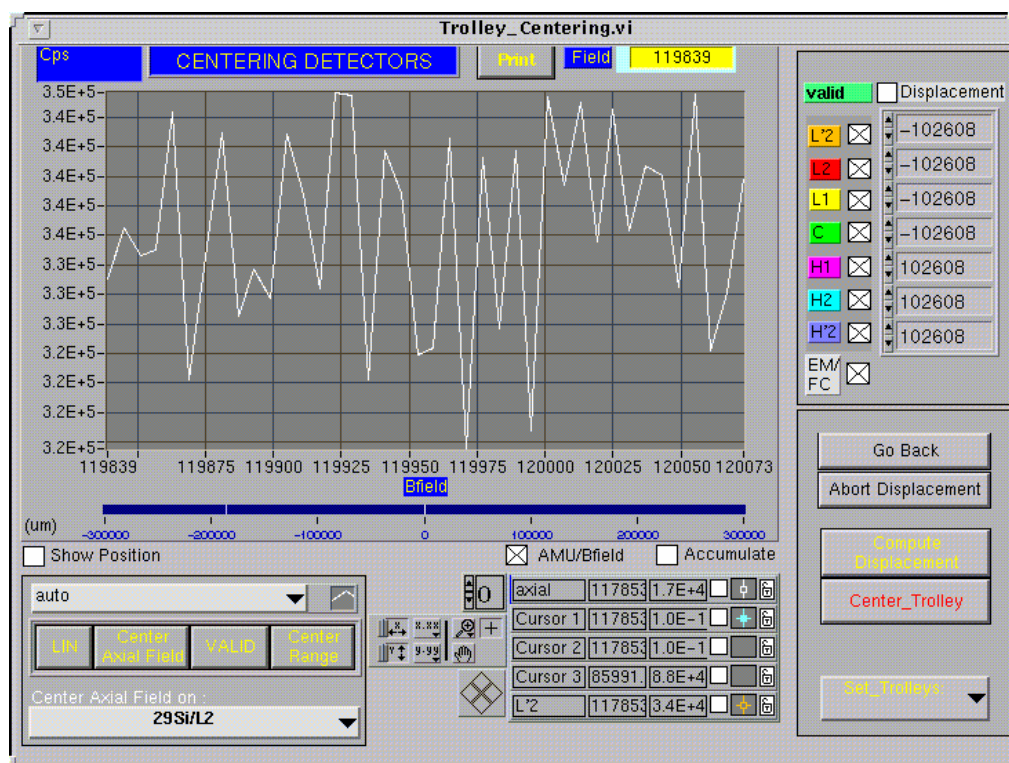
The B field is scanned over a range determined in the same way as for Mass Calibration (See the hereunder section § The Semi-Auto *MASS CALIBRATION*). When scanning the B field, there will be as many spectra as selected (crossed) detectors in the box located at the right side of the window.

When opening this window, all the cursors are at the plot center. Each cursor corresponds to the spectrum of the same color.

Center axial field for centering the *axial* white cursor onto the *axial detector* peak. The *axial detector* is selected in the field *center axial field on* .

center axial field on for selecting the detector which is considered as the *axial detector*. Such a selection is relevant so far the selected detector is actually located near the main axis.

VALID shift the current B field to the value indicated by the white cursor. In case of *ReStart*, the scan field will be centered onto this current B field.

Center Range allows to centre the B scan onto the axial cursor. If only a part of the peak appears in the graphics window, move the axial cursor towards the peak and click *Center range*. Nothing will be changed in the [m, b] table, but the peak will be contained within the B scan.

Center Field Automatic centering of each cursor onto the corresponding peak.

Center Trolley Each trolley, if checked in the *displacement* column, is moved to the position corresponding to the cursor (The formula *X=f(ΔM)*, displayed above in the section § *[The distance/mass multicollector metrology](#)* is used for this positionning).
WARNING: *Enable Centering*, in the right side box, is required to be clicked before *Center Trolley*

displacement displays the targetted positions if clicking *Center Trolleys*. Checkboxes are for validating the trolleys which would be actually moved.

Compute displacement displays in the columns the positions which will be targetted if clicking *Center Trolleys*.

***Set Trolleys (load position from file/ save position to file/ compute position*)** opens the *[Multicollector position library](#)* box for *load position* and *save position*, and opens the *[Compute position](#)* box in the last case.

<small>***Back***</small> After clicking *Center Trolley*, *Back* recalls the previous trolley positions.

Abort displacement aborts the moving in progress.

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4.4.6 The Collector Position Calibration process

In a simple case, all the masses are measured simultaneously, at the same fixed magnetic field. In the more general case, the multicollection analysis definition contains several subsets of masses required to be analysed at the same step of the magnetic field cycle.

1st Case: All the masses are measured simultaneously

The operator must first achieve a **coarse positionning** with the help of the *Muticollector Tuning* panel, the *Multicollection Control* dialog box and the *Multicollection Control Compute* box.
- In the main *Tuning* panel, set the Mass (or the B field) corresponding to the *main axis*.
- In the *Muticollector Tuning* panel, it is possible to view the coarse detector positions, measured either in microns, or in amu, providing that the metrology initialization has been previously achieved (<small>INIT</small> in the *Multicollection Control* dialog box).
- In the *Main Tool bar menu*, click <small>MULTICOL</small> for opening the *Multicollection Control* dialog box.
- In the *Multicollection Control* dialog box, click *compute pos* for computing the collector required positions.
- For each detector, the mass to be measured may be entered, and the *Compute* box computes the trolley position which can be transferred in the *Multicollection Control* dialog box.

Once the coarse positionning is achieved, the operator must launch the Multicollection Scan routine in order to get a **fine positionning**.
- From the *[main Tuning](#)* panel, click <small>CALL CALIB</small> for opening the *[Mass Calibration panel](#)* .

- Set *MRP*. Taking into account that the coarse positionning precision corresponds to ΔM/M=±1/1200, It is recommended to set MRP to 600 in order to get all the peaks within the scanning field.
- Click *TROLLEY CENTER* for running the scan and opening the *Multicollection Trolley Centering* panel.
- Select the detectors which must be calibrated in this run.
- Shift the cursors onto their peaks, accordingly to the guidelines described in the above section § *The Multicollection Center Trolley panel*.
- Move the trolleys to the cursor positions by clicking Center Trolley.
- Then increase the *MRP*, and *TROLLEY CENTER* again.

General case: The Multicollection analysis is achieved in a magnetic field switching mode.
Then, all the masses to be measured are divided into subset, each subset corresponding to the same magnetic field. Each subset masses will be measured simultaneously. It must be clear that during the analysis, only the magnetic field will be switched, while the collectors are not allowed to move. So, the procedure in this general case is the following:
- Set the positions of the first subset detectors, accordingly to the above described *first case*.
- Set the positions of the second subset detectors in the same way
- etc...

WARNING: If the same detector is used in several subsets, move it only at the first subset calibration. At further steps, a magnetic field tuning must be used for centering this detector peak.

> Before running a switching mode multicollection analysis, a Mass Calibration must be performed, accordingly to the guidelines given below in the section § *Calibrating the magnetic field before the analysis*.

5. Defining and Running an isotope analysis

5.1 Overview

For measuring isotope ratios of a given sample with the monocollection mode, the operator must have first edited an analysis definition file which contains the input data of an analysis: Species to be analysed, counting time for each species, ratios which are normally computed etc... This is described below in the hereunder section § *Defining an isotope analysis*.

Let us suppose that the instrument is started and tuned as it was explained above in the sections § *Starting the instrument* and § *Checking the instrument before an analysis*

Before running an analysis, it is first necessary to carry the right point of the right sample at the good location, at the cross point of both primary and secondary axis. (see § *The Sample Holder and Navigator* in the user's manual (2))

Then the operator will recall the analysis definition file if it is not the current analysis file, and normally, so far the analysis requires high mass resolution, it will be necessary to achieve a mass calibration in order to assign a precise magnetic field to each species. Due to

the magnet hysteresis, this operation must normally be repeated each time the instrument is out of the cycle of the analysis. See the hereunder section § *Calibrating the magnetic field before the analysis* .

The instrument is then ready for <u>starting an analysis</u>. see below the section § *Running an analysis*.

The analysis produces an <u>output data file</u>. For obtaining relevant results, the user can use some processing facilities such as the <u>isotope spreadsheet</u> . See the section § *Processing the results with the isotope spreadsheet* in the user's manual (2).

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5.2 Defining an isotope analysis

5.2.1 Overview

The operator may edit an analysis definition file for running it later or for running it immediately.

Editing and saving an analysis definition file
From the main menu bar, click *analysis definition* for opening the *ANALYSIS DEFINITION* box.
In the *ANALYSIS DEFINITION* box
- Select *ISOTOPES* as *Acquisition Mode*
- Click *EDIT LAST CONDITIONS* or *Load Conditions* or *New* for opening the *Species Table* dialog box.
- Enter the analysis input data (masses, counting time...) in the *Species Table* dialog box.
- Click on *save* or *save as* for saving the analysis definition file.

For running an analysis
In the *ANALYSIS DEFINITION* box
- Select the required analysis file
- Launch the mass calibration by clicking *CALIBRATE*
- After the mass calibration (quit the box calibration), click *APPLY* for opening the *ANALYSIS CONTROL* box.

In the *ANALYSIS CONTROL* box
- Click *START*

<div align="right">Contents ↑</div>

5.2.2 The *ANALYSIS DEFINITION* panel

This pannel can be opened from the *main menu bar*.
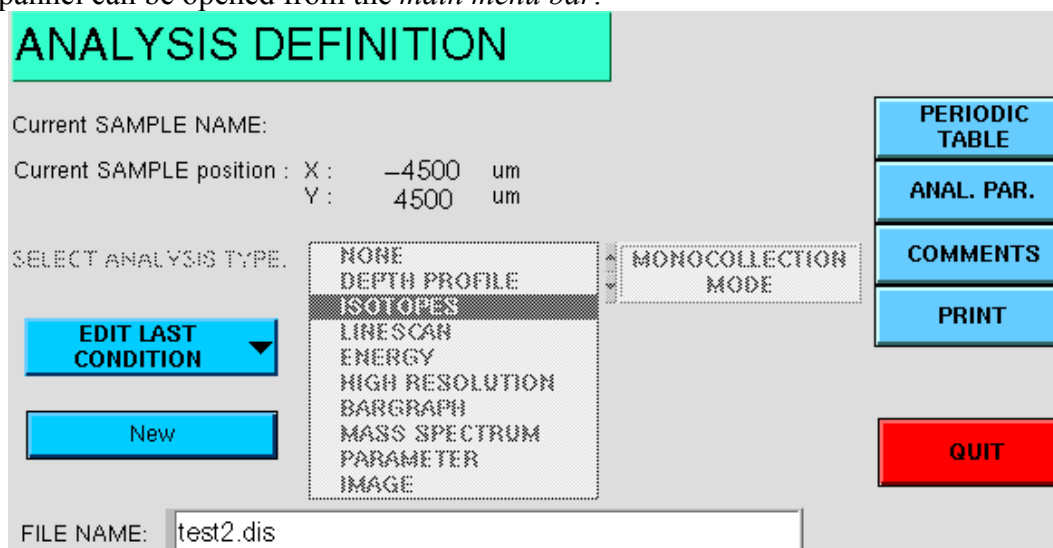
***MULTI/MONO* Mode** The selection of Multicollection mode allows to select a multicollector detector in the dialog box table while "Monocollection mode" restrict the selection to "EM/FC/FC2"

***SAMPLE NAME*, *SAMPLE X* DISPLAY Field**. The displayed data are generated by the "Navigator" (See the section § *The stage Navigator (HOLDER)*)

ANALYSIS TYPE
It selects the suitable dialog box, according to the analysis, and filters the displayed files according to selected acquisition mode

Avalaible acquisition modes	Mono/ Multi	Analysis file extension
Depth profile	both	.ddp
isotopes	both	.dis
lines scan	both	.ls
energy	both	.en
high resolution	both	.ddr
bargraph	mono	.
mass spectrum	mono	.
image	mono	.
Parameters	both	

File...: EDIT LAST CONDITIONS/ Load Conditions/ Save Conditions/ Save as/ New
opens the *SPECIES TABLE* box in the cases *Edit last conditions* or *New* , opens the *file dialog box* in the cases *load conditions* or *save* or *save as*.

New opens the ***SPECIES TABLE box***.

***FILE NAME* DISPLAY Field** name of the current analysis file

PERIODIC TABLE calls the *Periodic table* tool. See the section § *Periodic table* in the user's manual (2).

Analytical Parameters opens the box *Analytical Parameters*. The set of *Analytical Parameters* gives an overall information of the instrument setting during the analysis. This list will be included in the analysis output data (See the hereunder section § *Analytical Parameters*). Some of them are read on the instrument. Other are entered by the operator. These last parameters will be attached to the analysis definition.

COMMENTS `Edit Field` Comments to be attached to the analysis definition file. They will be printed with the analysis definition field

QUIT
Back to the main menu bar

Contents ↑

5.2.3 Analytical parameters

This table contains editing fields related to the status of the instrument hardware. Some values are directly read when the button *READ* is clicked.

WARNING, this program calls a 68030 µP routine which is actually not well-suited to the IMS1270. Some display fields are irrelevant or wrong (Transfer lens, field aperture)

All these parameters will be included in all the analysis output data files. Some of them are read and are targetted to record the status of the instrument hardware during the analysis. Other are filled by the operator.

The analysis does not depend at all on what the operator has written in this box. All of this information is considered as comments.

	EDITED/READ		EDITED/READ
Ion Species	Edited	Sample HV	READ
Primary HV	READ	ESA inner	READ
Arc Current	READ	ESA outer	READ
Primary cur beg.	MEASURED (1)	Transfer lens	READ (2)
Primary cur end	MEASURED	Gate DTOS	EDITED
Raster size	EDITED	Gate SII	EDITED
Primary beam size	EDITED	Entrance slit width	EDITED
HR aperture	EDITED	Energy slit width	EDITED
L4 aperture	EDITED	Mass Resolution	EDITED (3)
Duo pressure	READ	Anal pressure	READ
		Cont aperture	EDITED
		Field aperture	EDITED (4)

(1) The *Primary current beg.* and *Primary current end* fields display the primary current measured values, respectively at the beginning and at the end of the last analysis.

(2) The *Transfer lens* field displays always "35µm" which is irrelevant for an IMS1270.

(3) The *Mass Resolution* field is the single field with a (slight) action: For a new analysis definition, the *Mass resolution* column of the species table will be filled by default with the Mass Resolution written in *Analytical parameters*

(4) Not suited for an IMS1270: possible selection is 1/2/3/4 while 5 presets are available with the IMS1270.

READ activates the reading
SET copies the mass resolution to the new species table
EDIT

Contents ↑

5.2.4 The *SPECIES TABLE* box

This box is purposed to edit the analysis recipe; The analysis process consists of a given number of identical cycles. During each cycle, the magnetic field will be swiched to the values resulting from the mass calibration. Each field step consists of a waiting time targetted to allow the magnet to settle and a counting time.

All the table fields are editing fields except the *Mass* ans the *B field* columns.

GO TO ACQUISITION calls the main *Analysis Control panel*.

CALIB calls the *Mass Calibration panel*

CANCEL Closes the panel without saving the modifications.

Contents ↑

5.2.4.1 The species table in the monocollection mode

Main table

All the columns are `Edit Field`, except the columns Mass and B Field.
A line can be suppressed by deleting the species label and pressing ENTER.

Symbol	Species to be analysed; Possible formats: "*130.5*" ; then the calculated mass will be 130.5 "*Si*" ; then the calculated mass will be the Si major isotope exact mass: 27.9769 "30Si2 B" ; then the calculated mass will be 2*29.97649 + 11.00931 "30Si++" ; then the calculated mass will be 0.5*29.97649 The number of atoms for a given species is limited to 99 and a molecular isotope cannot contain more than 4 different isotopes.
Mass	`Display Field` (the value, in Dalton is calculated as described above)
Detector	EM/FC1/FC2
waiting time (s)	`Edit Field` If *Manual* is selected in the Analysis Definition box Default value 0.5 `Display Field` If *Auto* is selected in the Analysis Definition box, automatically computed according to the formula $$wt = \frac{\Delta B}{100000} * \sqrt{\frac{MR}{300}} + 0.1$$ An additional waiting time is edited in the right top corner for taking into account the FC settling time.
Counting time (s)	`Edit Field`
Offset (Volt)	Sample HV voltage offset to be applied for this species. Must be comprised between -127 V and +127V
Resolution	Mass resolution, identical for all the species. By default, it will be the value edited in *Analytical parameters*. It must be approximatively (1.2 10^6/Exit slit width) where the width is expressed in µm. The mass resolution will determine the initial range in *mass calibration.*
B field	`Display Field`, is filled according to the current table [M, B] if the analysis definition is *new*, of from the analysis *[m, b]* table if analysis definition was loaded from a file. The *[m, b]* table results from the last mass calibration.
EM drift	The *EM Drift* routine, if it is selected (See the hereunder section § *Additional Isotope boxes*) will be launched for the checked species. See also the § *EM Drit control*

If required, the lines can be scrolled with the button located at the top left side of the table. The number displayed besides the scrolling button is the number of the first displayed line.

The ISOTOPIC RATIO table

This *read only* table displays all the isotope ratios which will be normally computed in real time during the analysis and listed in the output spreadsheet. The table two columns correspond respectively to the ratio numerator and denominator which are edited by the *ratio defining box* (See the hereunder section § *The ratio defining box*). Both of them are linear combination of the measured species which can be edited by the means of the *define ratio* box which appears when clicking *define ratio*.
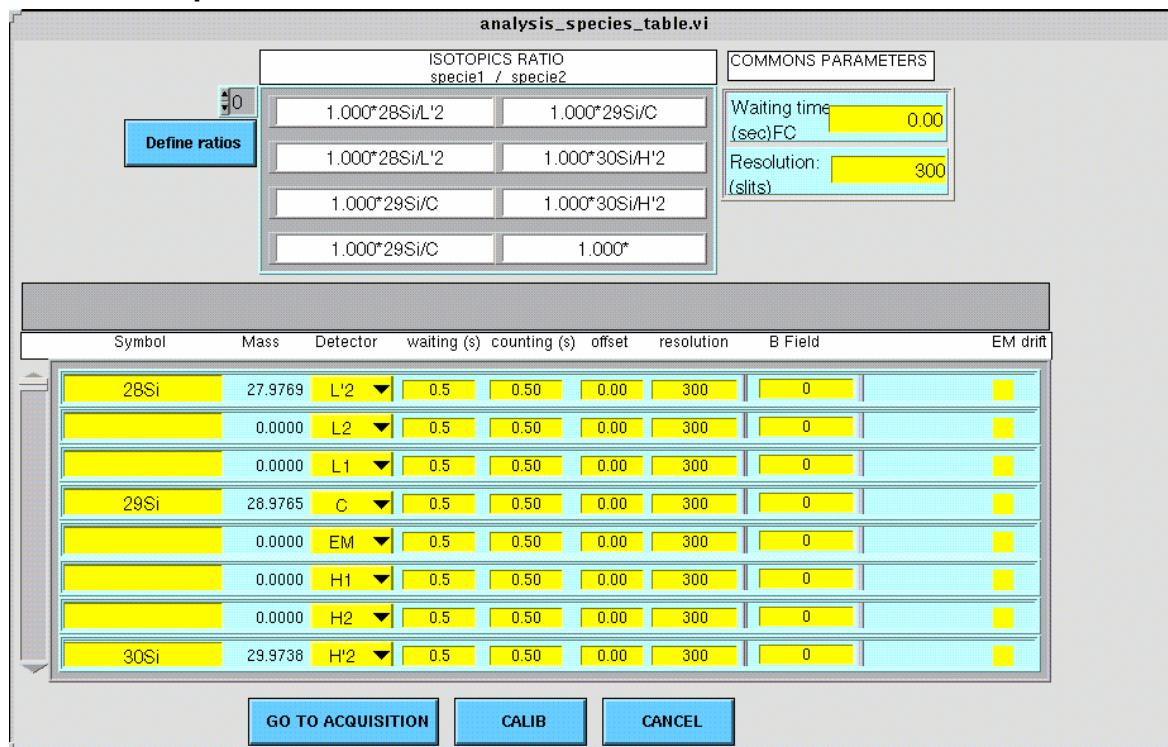
The COMMON PARAMETER table

FC Waiting time, `Edit Field`, is the additionnal waiting time concerning the species to be measured with a FC mode. It depends on the required precision and on the FC amplifier resistor. Typically, for a required precision of 2 10^{-4} and a resistor of 10^{11} ohms, it must be set

to 10sec. (See the appendix 4 § *The Faraday cup Measurement principle* in the user's manual (3))

5.2.4.2 The species table in the multicollection mode

analysis_species_table.vi

	ISOTOPICS RATIO specie1 / specie2		COMMONS PARAMETERS

Define ratios — 0

1.000*28Si/L'2	1.000*29Si/C
1.000*28Si/L'2	1.000*30Si/H'2
1.000*29Si/C	1.000*30Si/H'2
1.000*29Si/C	1.000*

Waiting time (sec)FC 0.00
Resolution: (slits) 300

Symbol	Mass	Detector	waiting (s)	counting (s)	offset	resolution	B Field	EM drift
28Si	27.9769	L'2 ▼	0.5	0.50	0.00	300	0	
	0.0000	L2 ▼	0.5	0.50	0.00	300	0	
	0.0000	L1 ▼	0.5	0.50	0.00	300	0	
29Si	28.9765	C ▼	0.5	0.50	0.00	300	0	
	0.0000	EM ▼	0.5	0.50	0.00	300	0	
	0.0000	H1 ▼	0.5	0.50	0.00	300	0	
	0.0000	H2 ▼	0.5	0.50	0.00	300	0	
30Si	29.9738	H'2 ▼	0.5	0.50	0.00	300	0	

GO TO ACQUISITION   **CALIB**   **CANCEL**

With the multicollection mode, the analysis definition is sligthly more sophisticated since, additionally to the magnetic field values which must be successively switched at each field step, the analysis definition file must also contains which detector will be used for each specie. Consequently, the species table consists of different subtables, each subtable corresponding to the species subset which will be measured simultaneously at each field step. The scroll button at the table top left corner allows to switch from one subtable to another one.

Each species subtable contains the 7 lines corresponding respectively to a particular collector L'2/L2/L1/C/Main/H1/H2/H'2 which are displayed in the column *Detector*. According to the *detection set-up*, which must be updated by the operator whenever a detector FC or EM is switched on a moving collector (See the section § *Detection setup* in the user's manual (3)) the instrument is aware of which detector is mounted onto a given moving collector. For the fixed *Main* collector, the operator must select the detector FC1/FC2/EM, since the 3 detectors are always mounted and available.

In a given subtable, the *waitingtime*, *counting time*, *offset*, *resolution* and *B field* columns accept a single value. Editing any line will automatically set all the column to this edited value.

In the multicollection mode, if the option *from table* was selected in the *Analysis definition* box (instead of *from condition*), the column *B field* is an `Edit Field`. The reason is that, at this stage of operation, the instrument was not yet given the data of the collector locations. So, it cannot deduce which mass will correspond to the main axis, and then, which magnetic field B can be interpolated from the table [M, B]. Q26

So, the first time a multicollection analysis is defined, the operator must estimate for each subset the mass corresponding to the main axis. If the trolley settings were performed as described above in the section § *Multicollection case: Setting the trolley positions*, for each subset, the tuning displays which value must be entered as B field, providing that *FIELD* is selected instead of *MASS*.

5.2.4.3 The ratio defining box

This box purposed to define the ratios computed with the analysis data can be opened previously to an analysis, from the *monocollection species table* or the *multicollection species table*, and in this case, these ratios can be displayed in real time along the analysis in the *Isotope Spreadsheet*. It can also be opened during or after an analysis in the *Isotope Spreadsheet* to define new ratios.

The box allows to edit the different coefficients c1, c2, c3... associated to each measured species for building respectively the numerator and the denominator in the form

$$c1*M1 + c2*M2 + c3*M3 ... +c0$$

Obviously, zero will be often choosen. Note that the possibility to set all the denominator coefficients to zero except c0 (set to 1) allows to display the intensity of one measured species in the output *Isotope Spreadsheet*.
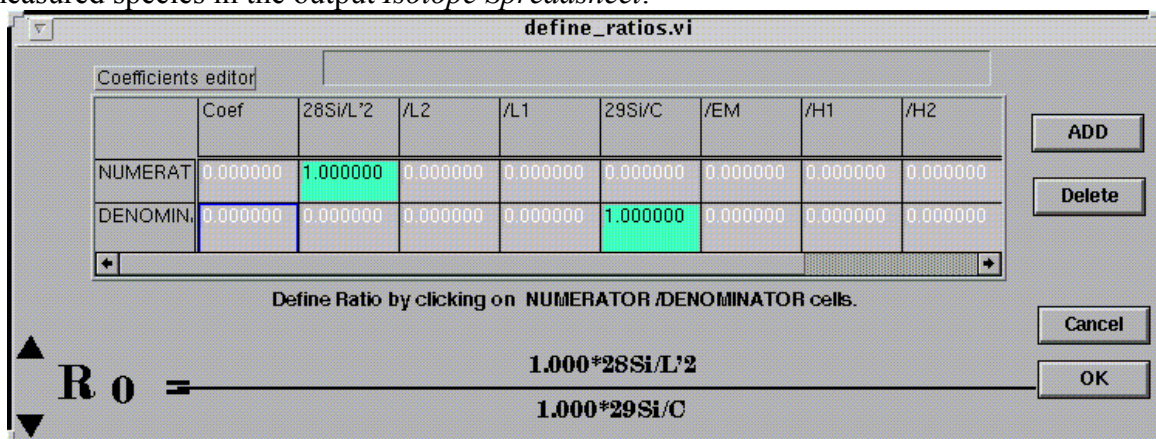
Add for defining a new ratio.
Delete for deleting the displayed ratio.
Cancel for closing the box without any modification.
OK for closing the box and saving the last modifications.

> It is possible but not necessary to define isotope ratios before running an isotope analysis.
> Isotope ratio can also be defined during or after the analysis

5.2.5 The additionnal ISOTOPE boxes

5.2.5.1 Overview

A single additional box is required to be filled for defining an isotope ratio since: The *Isotopes* box which is opened simultaneously with the *analysis species table* and defines the analysis timing. Other boxes are optional and may be selected from the *Isotopes* box.

1. Beam-Blanking	If this option is selected, the primary beam is set off (blanked) during the waiting time. This option is recommended when material must be saved.
2. Pre-sputtering	See the hereunder section § *Pre-sputering*
3. Reference Signal	See the hereunder section § *Reference signal*
4. Mass calib control	See the hereunder section § *Mass calibration Control*
5. HV sample control	See the hereunder section § *Sample HV Control*
6. Overlapping crater	See the hereunder section § *Overlapping crater*
7. EM Drift Measurement	See the hereunder section § *EM drift Control*
8. BEAM Centering	See the hereunder section § *Beam Centering*

Contents ↑

5.2.5.2 The *Isotopes* box: Analysis time, Cycles, Blocks

ISOTOPES

ANALYSIS TIME: (s) `75`

CYCLE NUMBER: `100`

BLOC SIZE: (cycles) `20`

Rejection condition: `0`

BEAM BLANKING :
PRE-SPUTTERING ⊠ ...
REFERENCE SIGNAL ...
MASS CALIB. CONTROL ...
HV SAMPLE CONTROL ...
OVERLAPPING CRATER ...
EM/Drift Measurement ...
BEAN CENTERING ...

The isotope analysis cycle parameters

ANALYSIS TIME, `Edit Field`, is the total analysis time, in seconds, which will be further rounded off for consisting of an integer number of cycles. When the field *ANALYSIS TIME* is edited, the following field *NUMBER OF CYCLES* is computed taking into account the waiting time and the counting time selected for each species, and displayed. Reversly, if the field *NUMBER OF CYCLES* is edited, the field *ANALYSIS TIME* is computed and displayed.

NUMBER OF CYCLES , `Edit Field` is the total number of cycle. See above the interaction with *ANALYSIS TIME*.

BLOCK SIZE, `Edit Field` is a number of cycles smaller than the total number of cycles. The analysis will consist of an integer number of blocks. In the isotope spreadsheet, , the data will processed in real time block per block. It will be possible to modify the block size in the post-processing mode.

Rejection condition, `Edit Field` is a parameter of the statistical analysis which is achieved in real time. See the spreadsheet documentation. Enter *0* for no rejection, and 3, for example for a rejection at 3 σ.

At the box bottom, ckeckboxes allow to select analysis options. Except the first option (*Beam-Blanking*), other options are additional routines which can be included within the analysis timing.

If these options (2/3/4/5/6/7/8) are selected, clicking the text button opens the dialog box purposed for entering the option input data.

Contents ↑

5.2.5.3 Isotope analysis option (2): Pre-sputtering
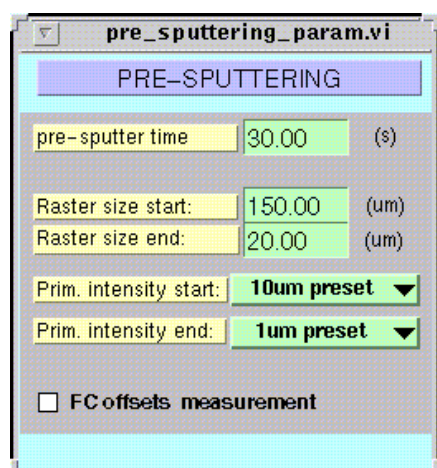
This option is recommended for ensuring the analysis will start once the secondary emission steady state is reached.

If this option is selected, the sample is sputtered during *pre-sputter time* before this analysis.

During the *pre-sputter time*, the Raster size is *Raster size start* while during the analysis, it will be ***Raster size end*** .

In the same way, the primary current preset can be different during the sputtering time (***Prim. intensity start)*** and during the analysis (***Prim. intensity end)***

5.2.5.4 The isotope analysis options (3): Reference signal

Not very helpful for isotope analyses

If this option is selected, a species must be entered in the *reference signal* dialog. This species secondary signal is then measured at the end of the analysis and stored in the raw data file.

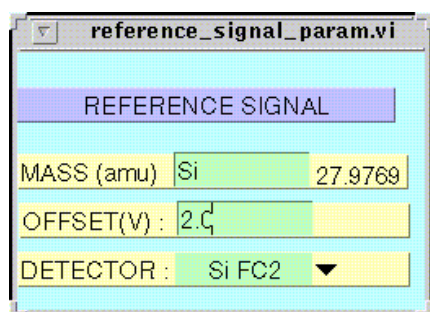### 5.2.5.5 The isotope analysis options (4): Mass calibration Control

This option is recommended for long High Mass Resolution analyses.

The *Mass Calibration Control* consists of recording during the analysis a narrow mass spectrum centered onto the mass species specified in the dialog box *Mass calib control*. This mass species must be contained in the main species table of the analysis. New automatic mass calibrations will be achieved during the analysis for this mass each n cycles (n being the data entered in the field *period*); all the species table magnetic field values will be then corrected by the same relative variation if only one species is specified to be recalibrated. Note that several species can be specified to be recalibrated. In this case, the relative variation is interpolated between 2 recalibrated masses.

When the *Mass Calibration Control* routine is being run, a panel is displayed and the operator may take the priority, if required (See the hereunder section § *The auto-centering panel*), though the *Mass Calibration Control* routine is firstly targeted to be run without any operator action.
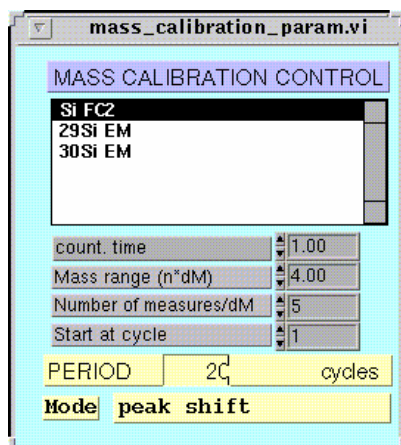
period, the number of cycles between 2 mass calibration is edited in the field *PERIOD*. The field *cycle numb* edits the cycle number of the first in-analysis mass calibration

Count.time,*#meas./dM*, *mass range*, *cycle numb* are the mass calibration parameters (see the hereunder section § *The Semi-Auto MASS CALIBRATION panels-1: The main window*)

The list of the ΔB computed at each mass calib control is included in the raw data analysis output file.

2 modes, *peak shift* and *peak centering* are available.

The *peak centering* mode

This mode involves the standard *center* algorithm used in mass calibration. It can be used provided that the species to be calibrated corresponds to the highest peak within the scanned range and that this peak is separated from other peaks in the area comprised between both sides Half Maximum points.

The actual *center* algorithm detects the maximum Y0 over the scanned range, then, respectively on the up side and the down side, the points (X1, Y0/2) and (X2, Y0/2), and the peak center is computed as (X1+X2)/2.

The *peak centering* mode is run entirely automatically.

The *peak shift* mode

This mode is required whenever the *peak centering* mode cannot be used. It cannot be run automatically since the operator must set the output B value with the cursor onto the first mass calib control mass spectrum.

This first mass spectrum is recorded, and the next mass calib control will involve a standard correlation function algorithm for computing the shift between the first recorded spectrum and the new spectrum.

5.2.5.6 The isotope analysis options (5): Sample HV Control

This option is recommended for long analyses onto insulating and metallized samples when using O⁻ and positive secondary Sample HV.
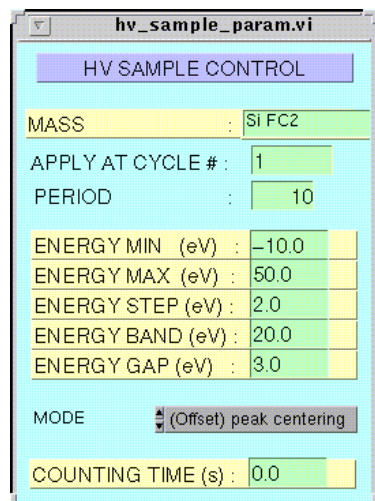
2 modes are available: *Offset correlation* and *Offset centering*. Other modes (*slit correlation*...) which appear in the dialog box are not working. Both modes consist of checking the energy distribution, and if a shift is detected, to give the sample HV an offset in order to cancel the shift which was measured.

To understand the *Sample HV Control*, it must be clear that the secondary ion beam is dispersed in energy by the main ESA, and if the sample HV is therefore scanned while the energy slit is set to a narrow width (<1eV), the resulting curve I(Sple HV) is the secondary energy distribution curve of the considered species.

When the sample HV is scanned with a rather large (25eV) energy slit width - *that is the case with the Sample HV Control process* - the recorded curve is not exactly the energy distribution curve, but the energy distribution convoluated by the energy slit width. Nevertheless both correlation and centering modes are using this curve to recenter the energy distribution with respect to the energy slit position.

The list of the ΔV computed at each Sample HV control is included in the raw data analysis output file.

When the *Sample HV Control* routine is being run, a panel is displayed and the operator may take the priority, if required (See the hereunder section § *The auto-centering panel*), though the *Sample HV Control* routine is firstly targetted to be run without any operator action.

The *Offset centering* mode

This mode can be used only if the Energy Slit width is larger than the edited *Gap*.

Taking in account what is explained above, it must be clear that the curve displayed on this section figure is the <u>virtual</u> energy distribution curve, which would be displayed if an energy spectrum was recorded with a very narrow energy slit.

Note that the *Offset centering* mode is run entirely automatically.

Sample HV Control dialog box (`EditING FieldS` **)**

MASS	A reference species . It must belong to the list of species analyzed in order to keep the same cycling sequence of the magnet for the overall analysis.
APPLY AT CYCLE #	The number of the cycle for the first sample HV calibration control. The control procedure is executed at the beginning of this cycle.
PERIOD	The period N (entered in number of cycles) of the sample HV calibration control .
ENERGY MIN (eV)	*Offset min.* : the low limit of the offset range to be scanned in order to record the reference energy distribution.
ENERGY MAX(eV)	*Offset max.* : the high limit of the offset range to be scanned in order to record the reference energy distribution.
ENERGY STEP (eV)	The offset s*tep* to record the energy distribution.
ENERGY BAND	The *energy pass band* of the mass spectrometer which is controlled by the energy slit width.
ENERGY GAP (eV)	The *energy gap* : it is a gap left between the beginning of the energy distribution and the low energy side of the energy slit.
MODE	*(Offset) peak-centering/ Offset Correlation*
COUNTING TIME (s)	The *counting time* per data point to record the reference energy distribution.

Sample HV Control Procedure in the offset centering mode

The analysis starts. When the cycle previous to the cycle selected to carry out the first sample HV control is completed, the magnet field cycling goes on, complying with the waiting times but not with the counting times on different species, until the reference species is reached.

While being on the reference species, the sample offset is scanned from the low limit to the high limit entered by the operator. For the scan, the offset is added to any offset value already applied provided that the sum remains lower than 127 V. A reference energy distribution is recorded. During the acquisition, this energy distribution can be displayed in a window of the *analysis control* program .

The program determines the offset value corresponding to the maximum of the energy distribution V_{off}(max.), and then the offset value V_{off}(5%) yielding to 5% of the maximum intensity measured towards the low energy side of the energy distribution. The new sample HV offset value applied to go on the analysis is computed with the relationship :

$$V_{off} = V_{5\%} - \left(E_w - E_{gap} \right) \text{ for positive secondary ion analysis.}$$

$$V_{off} = V_{5\%} + \left(E_w - E_{gap} \right) \text{ for negative secondary ion analysis.}$$

The acquisition re-starts with the new sample HV offset value applied until the next control .

The V_{off}(new) values determined during the acquisition can be displayed in a dialog box of the *analysis control* program. They are saved in the raw data file at the end of the analysis.

The energy distribution centering routine

The illustration shown in step #0 shows the status of the energy distribution centering before the sample HV control. It is not correct because the low energy side of the energy distribution is stopped by the low energy edge of the energy slit.

The illustrations shown in step #1 and step #2 correspond to an analysis of positive secondary ion analysis. In case of negative secondary ion analysis, in step #1, the offset voltage would be equal to V(old)+ offset max. and V(old)+ offset min. in step #1 and step #2, respectively.
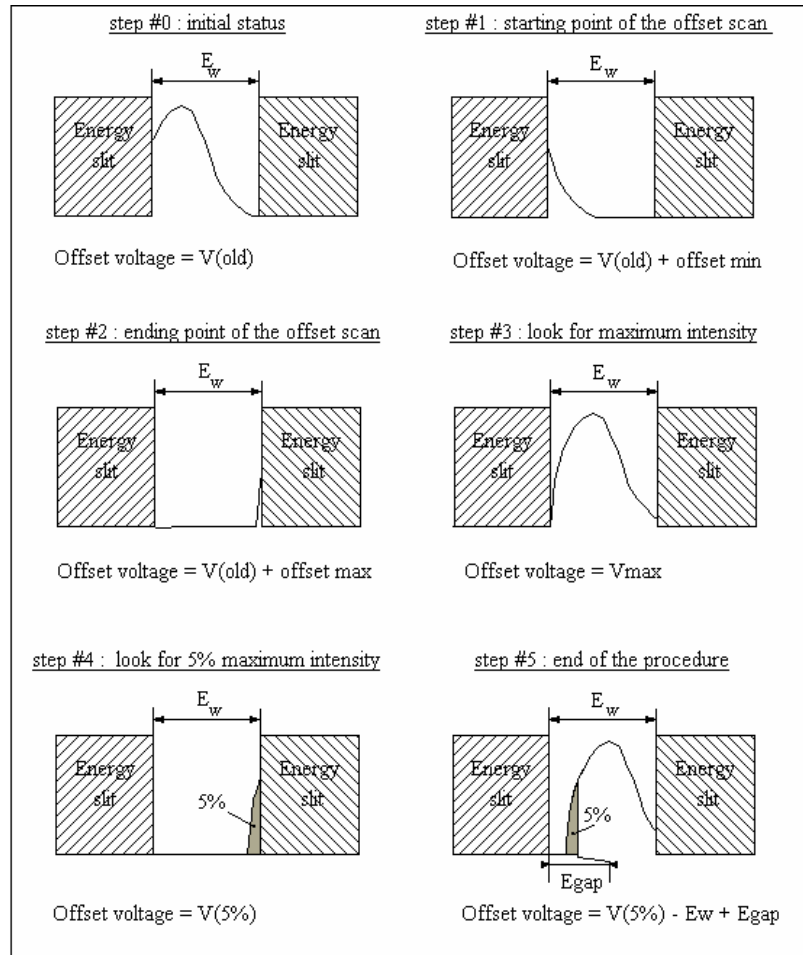
The *Offset correlation* mode

With the *Offset correlation* mode, the process compute the shift between the first control curve and the current control curve. This mode is required whenever the required *Gap* would be larger than the slit width. It cannot be run entirely automatically.

The dialog box *Gap* field is not used. It is replaced by an interactive mode after the first control which occurs normally before the analysis (set *APPLY AT CYCLE#* at 0. The operator must then use the cursor to set the first sample HV offset. This first recorded curve will be used as a reference curve.

Further, at each Sample HV Control, the shift between the reference curve and the new recorded curve is computed with a standard correlation function algorithm and it is substracted from the previous sample HV offset.

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5.2.5.7 The isotope analysis options (6): Overlapping crater
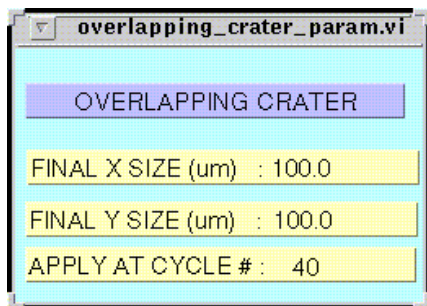
For this function, use the pre-sputtering option

5.2.5.8 The isotope analysis options (7): EM drift Control

This option is recommended whenever the Em is suspected to drift or whenever it is important to check it does not drift
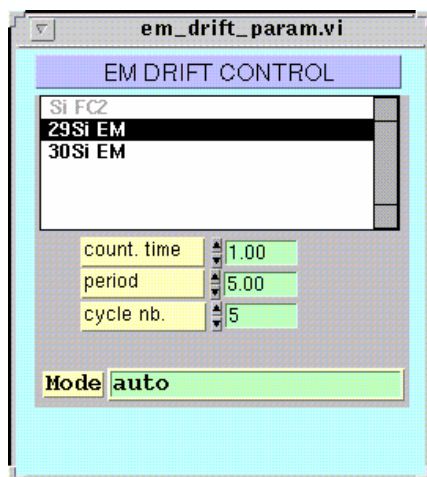
The *EM Drift Control* Routine is run every **cycle nb** cycle. (See the decription of this routine in the section § *Em Drift Measurement Description* of the user's manual (2))

Count. time and ***Period*** are the routine parameters, as they are defined in the measurement parameters box (See the decription of this routine in the section § *Set Thresholds for the PHA featuring routine* of the user's manual (2). In the *Set Threshold* boc, "period" is labelled "#cycle")

Mode Auto/Manual The routine is run automatically if *Auto*, and stops at the *EM Drift Control* panel if *Manual*. The operator may then change some parameters and must click *Start*)

5.2.5.9 The isotope analysis options (8): Beam Centering

This option is recommended whenever the analysis is included within a *chained analysis* with large stage motion between different analysis points.
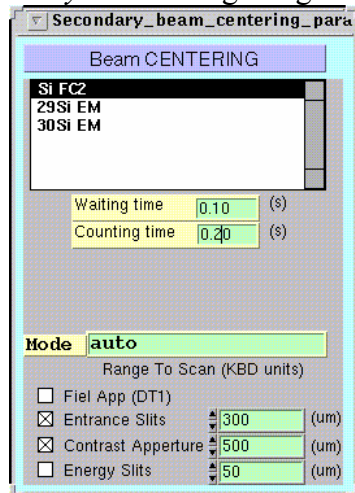
The *scan parameter* Routine is run at the analysis beginning, just after the presputtering, successively for The DT1 X&Y Centering, for the Entrance Slit (X-axis), the Contrast aperture (Y-axis) and the energy slit (X is scanned, W is constant) (See the decription of this routine in the above section § *Scan parameters*)

waiting time and *counting time* corresponds to the *waiting time* and the counting time of the *scan parameter* panel.

Mode auto/manual The routine is run automatically if *Auto*, and stops at the *scan parameter* panel if *Manual*. The operator may then change some parameters and must click *Start*)

5.3 Calibrating the magnetic field before the analysis

5.3.1 Introduction

5.3.1.1 The mass calibration issue

The mass calibration routine which is achieved just before starting an analysis is targetted to determine as precisely as possible the value B which will give the right mass M at the exit slit center.

The same mass calibration routine is used for setting the field B_i of the point (M_i, B_i) of the [M, B] table, but the output B_i fills the analysis species table and not the current [M, B] table.

> The *Mass Calibration* routine, when called from
> Analysis does not modify the current *[M, B]* table.

5.3.1.2 The M-B memory effect

It must be first emphasized that while M is the exact mass which is expected on axis at the exit slit plane, B is not the actual magnetic field within the magnet, which is not a single value, but a distribution along the main path. B is the input value sent to the servoed system which controls the magnet supply with the constraint that the difference between B and the Hall probe output measurement is zero.

For different physical reasons, magnet hysteresis, Hall sensor thermal effects, eddy currents, the mass M which results from adressing B to the magnet supply depends on the last $\{... B_{t-3}, B_{t-2}, B_{t-1}\}$ history.

The issue is to determine the value B which will set the required mass M onto the exit axis. The above memory effect produces an uncertainty onto the relationship B(M).

5.3.1.3 The cycling strategy

This last uncertainty is dramatically reduced when the same B serie (B_{min}, B_2... B_i,... B_{max}) is cycled, and providing that the successive B values are growing from B_{min} to B_{max}. After a few number of cycles, the value of the mass produced at the exit axis reaches a steady state, and its uncertainty can be reduced down to a few ppm.

Fortunately, it is possible to keep regular B cycles over an analysis. The mass calibration strategy consists therefore to calibrate the values B_i associated to the respective masses M_i while cycling B according to the analysis cycle and to avoid to get out of the cycle between the mass calibration and the analysis.

So far a high mass resolution is required, each time the analysis cycle is broken, the mass calibration must be performed again.

> From the Mass Calibration stage up to the end of the analysis, the instrument must be kept in the same analysis B field cycle

5.3.1.4 The *ANALYSIS MASS CALIBRATION* [m, b] table

The *ANALYSIS MASS CALIBRATION* routine involves a [m, b] table different from the current [M, B] table. This [m, b] table is initialized by the analysis species table. Along the mass calibration process, the b values are modified (but never the m values), and at the end of the process, the modified b values are sent back to the analysis species table.

In the multicollection case, "m" does not correspond to a given species, but to a subset of species which must be measured at the same time.

> The *Mass Calibration* defines the B to the magnet control system for each mass

5.3.1.5 Monocollection and Multicollection analyses

The main issue of a monocollection analysis is the memory effect. The solution is to record the successive high resolution peak spectra within a cycle in order to calibrate each mass B field.

Some multicollection analyses do not require magnet switching. In this case, the B field calibration consists just to achieve a single B field scan and to select the right static B field. But previously the different collectors required by the analysis must be correctly positionned. This issue is addressed in the above section *§ Checking the instrument before an analysis/ Multicollection case: Setting the trolley positions* . The *mass calibration* which simultaneously displays all the collector signals allows also to check the collector positionning.

The multicollection analyses which involve magnet switching will require a first stage of collector positionning and a second stage of B field calibration identical to the monocollection case.

5.3.1.6 Manual and semi-auto *Mass Calibration* modes

2 *Mass Calibration* modes are proposed to the operator:

- The *manual mode*, (previously labelled as *PUNCTUAL CALIBRATION*), invites the operator to tune manually the B field by means of the keyboard thumbwheel for each mass.
- The *semi-auto* mode, (previously labelled as *CALIB. AID MANUAL*), scans the B field for each mass, displays the spectrum and invites the operator either to set the B field by mouse driving a cursor on the spectrum or by using an autocenter routine.

5.3.2 Analysis *Mass Calibration* Overview

Let us suppose that in the multicollection case, the trolleys have been correctly positionned, accordingly to the procedure described above in the section § *Multicollection case: Setting the trolley positions*.

Either the operator has selected an analysis file from the main *ANALYSIS DEFINITION* box, and in this box, he clicks *MASS CALIB*, or he is already in the ANALYSIS with a current analysis file, and he clicks *MASS CALIB* in order to update the species table B field, the *MASS CALIBRATION* panel appears on the screen (See the panel in the hereunder section § *The Analysis MASS CALIBRATION* panel). The recommended procedure is as it follows:

- At a first step, the operator performs a coarse calibration. For this purpose, he must click onto *MASS CAL. MANUAL* . Then, the program switches successively the magnet at the B field values which are contained within the mass calibration [m, b] table. At this mass, the operator is allowed to play with the dedicated keyboard thumbwheel and to search forward the right value of the magnetic field by maximizing the bargraph signal level or by positionning the entrance slit image on the MCP camera image.
- At a second step, the operator performs a fine calibration by running the semi-automatic mass calibration. It is recommended first to run a few number of cycles (*CYCLING+ START*). Then, the operator must click *MASS CAL. SEMI-AUTO* and will be assisted for the search of the right B field: For each mass, a B field scan will be run and the spectrum will be displayed in a graphic window. The operator can then tune finely the B field by using an autocenter routine or positionning manually a cursor.
- Clicking APPLY will transfer the *Mass Calibration* [m, b] table towards the analysis species table, close the *Mass Calibration* window and open the *Analysis* Window.

During these both processes, a table displays the mass calibration status: Which mass has been still calibrated and which field is assigned to each mass.

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5.3.3 Manual Mass calibration

5.3.3.1 The *Analysis MASS CALIBRATION* panel

      The Analysis *MASS CALIBRATION* panel is displayed if *MASS CALI MANUAL* is clicked from the main *MASS CALIBRATION* panel. 2 other panels are opened as well, see the next section § *The Manual MASS CALIBRATION panels*

The Analysis Mass Calibration Panel with the manual calibration Bargraph
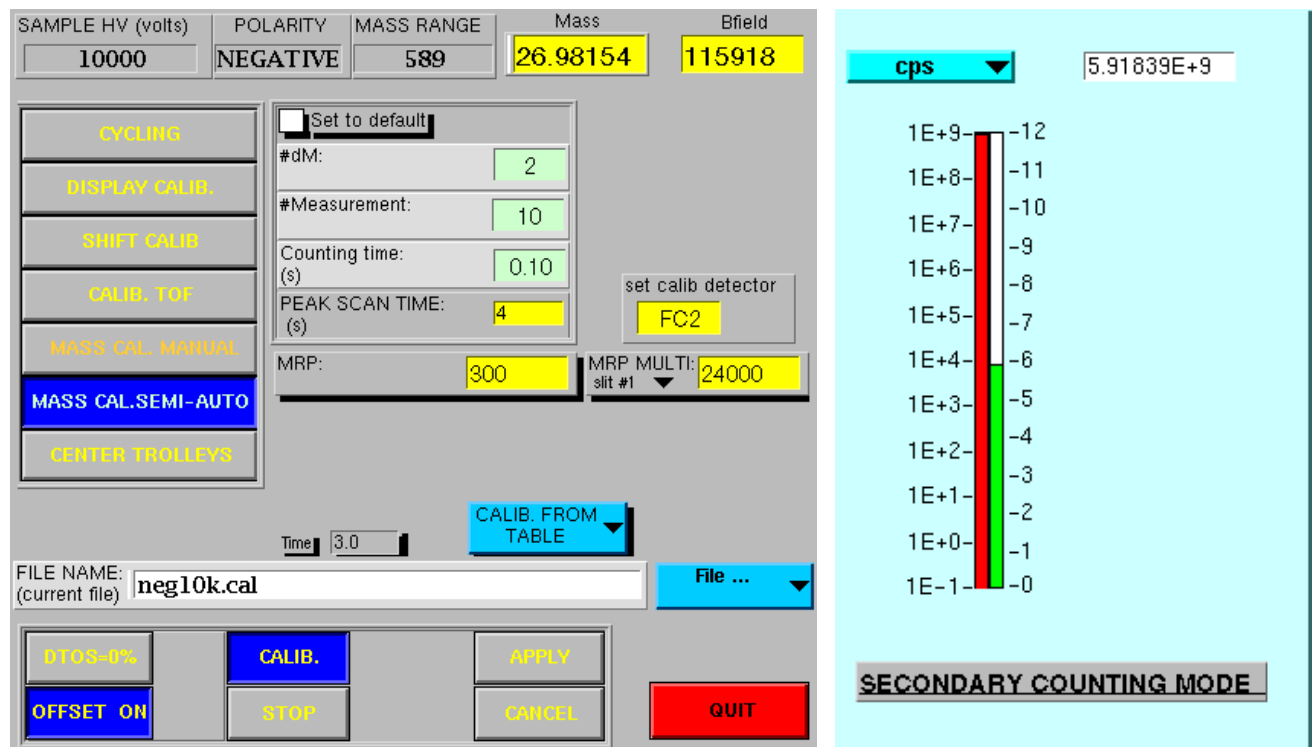
Top horizontal bar

SAMPLE HV , `EDITING/DISPLAY Field`, is the sample HV which was recorded in the current [M, B] table file when it was created.

POLARITY , `DISPLAY Field`, is the sample HV polarity which was recorded in the current [M, B] table file when it was created.

MASS RANGE, `EDITING/DISPLAY Field`, is the Mass Range which was recorded in the current [M, B] table file when it was created.

Vertical menu bar

 See the above section § *The Main MASS CALIBRATION Panel* for *DISPLAY CALIB* and *SHIFT CALIB* and *CALIB_TOF*.

CYCLING *(TAGGED/NOT TAGGED)* selection: When clicking *CYCLING*, it gets tagged in blue, and new buttons *START*, *STOP*, nb of cycles are displayed at the right top side of the window. *START* activates a mass cycling with the analysis timing. Nb of cycles, `EDIT Field`, must be used for programming a given number of cycles. In a fine calibration, it may be useful to run some cycles before the calibration to reach faster the steady state.

No calibration can be achieved when *CYCLING* is ON. *CYCLING* must first be stopped (Click the button *CYCLING* and it will no more tagged). Note that the dynamic cycle is always stopped, without broking but the B field cycling.

> If *CYCLING* is tagged in blue, any mass calibration cannot be performed

DISPLAY CALIB See the section § *The Main MASS CALIBRATION Panel*

SHIFT CALIB See the section § *The Main MASS CALIBRATION Panel*

CALIB_TOF See the section § § *Procedure for Calibration the TOF (Time of Flight)*

MASS CAL. MANUAL allows to perform a semi-auto calibration and opens the corresponding dialog boxes.

MASS CAL.SEMI-AUTO corresponds to the entirely automatic mode but has not yet been validated for the version 3.1

CENTER TROLLEYS Is used for the multicollector, once a given mass peak has been adjusted with respect to the corresponding detector, it allows to center mechanically the other moving detectors with respect to other ion peaks. See the above section § *The Multicollection Center Trolley Panel*

The bottom bar

START : If *MASS CAL. MANUAL* or *MASS CAL.SEMI-AUTO* is selected, starts the mass calibration process. The button is then labelled *CALIB*. The mass calibration [m, b] table is then filled by the species table values.

VALID must be clicked once the b_i field is correctly tuned for the current species m_i. This value b_i is then displaced to the [m, b] table, and the calibration process steps automativally to the next species m_{i+1}

DTOS (ON/OFF) enables ou disables the DTOS function.

OFFSET ON/OFFSET OFF If *OFFSET OFF* is selected, the sample HV offset listed in the species table are not loaded.

APPLY The calibrated fields b_i are transfered from the *Mass Calibration* [m, b] table to the Analysis definition file. The *MASS CALIBRATION* panel is closed, and back to the panel *ANALYSIS*.

STOP The Mass Calibration process is immediately stopped and the B cycle can therefore be broken. The mass calibration [m, b] table may then be transferred to the analysis mass species table by clicking *APPLY*, or a new mass calibration process may be started by clicking *Start* . This new process will then be intitialized by the current mass calibration [m, b] table (as it was when clicking *STOP*).

The scan parameters at the panel center

#dM, `EDIT Field,` defines the half number of *peak width* to be scanned. The peak width, if expressed in B field digits is equal to 2*B/MR. Note that the peak width is actually equal to B/MR if the Mass Resolution MR entered for the analysis is equal to K/(*Exit slit width*), the mass dispersion coefficient K being equal to 1210000 μm for the IMS1270.

$$scan\ width = (2*B/MR) * (\#dM)$$

Default value: #dM=4

MR is the value displayed in the field *MRP* (See above, the section § *The Analysis MASS CALIBRATION panel*)

#Measurement, `EDIT Field,` is the number of points which are stepped within one peak width. This leads to the rounded step between 2 points, in B field digits and to the total number of points.

$$Step = \text{rounded}((2*B/MR) /(\#Measurement))$$

Default value: #Measurement = 11

If *Max* is crossed, the scan will step at all the magnetic field digits.

Counting time, `EDIT Field,` is the counting time per points, expressed in seconds.
Default value: 0.2 sec

PEAK SCAN TIME, `DISPLAY Field,` is the scanning time of the currently displayed mass, resulting from the other 3 field data:

$$Peak\ scan\ time = (\#dM) * (\#Measurement) * (Counting\ time)$$

Checking **set to Default** gives the above parameters their default values.

Other fields

FILE NAME, `DISPLAY Field,` is the name of the current [M, B] table file.

File (load/ save/ save as/ Init new file/Init new file /file info allows to load and save a *[M,B]* table. See the *file dialog box* in the above section § *The Main MASS CALIBRATION Panel*

MRP, `EDIT Field,` is the *Mass Resolution MR*, to be defined by the operator. When opening the *Mass Calibration* window, the displayed value is the *Analysis Mass Resolution* if the *Mass Calibration* routine is called from Analysis or the last used value if it is called from tuning. This value determines the B field scan width.

CALIB.FROM TABLE/ CALIB FROM CONDITIONS This selection is used only when the *Mass Calib* is called from *Analysis definition*. Whenever *CALIB FROM TABLE* is selected the initial *Bfield* corresponding to each mass is derived from the *[B, M]* table. Whenever *CALIB FROM CONDITIONS* is selected the initial *Bfield* comes from the analysis *[m, b]* table. See the above section *The Mass Calibration [m, b] table*

Set calib detector (EM/FC1/FC2/L'2/L2...) selects the detector involved in the *Mass Calibration*.

Contents ↑

5.3.3.2 The Manual *MASS CALIBRATION* panels

The monocollection case

When Clicking *MASS CAL. MANUAL*, 2 panes are opened additionally to the main panel and to the bargraph

- The manual mass calibration table window
- A tuning window very similar to the main tuning window.

The manual mass calibration table window

	CALIB ?	DONE		Mass Symbol	Mass a.m.u.	B Field
0	YES	☐		Si	27.9769	117856
1	YES	☐		29Si	28.9765	119959
2	YES	☐		30Si	29.9738	122021
0	YES	☐			0.0000	0
0	YES	☐			0.0000	0
0	YES	☐			0.0000	0
0	YES	☐			0.0000	0
0	YES	☐			0.0000	0

All the above table columns are described below in the section § *The Semi-Auto MASS CALIBRATION panels-3: The mass calibration table*

The manual mass calibration tuning window
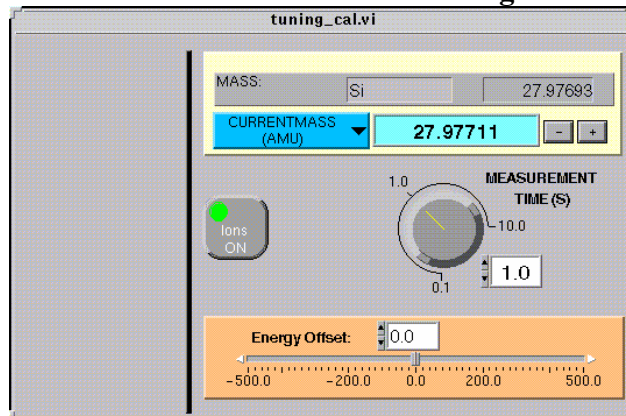
As it can be understood from this panel, the manual mass calibration tuning window can be used both for modifying the mass calibration counting time and the sample HV offset and for setting the B field.

The multicollection case

The multi-bargraph window is opened instead of the single bargraph.

5.3.3.3 The manual Mass Calibration process

- After clicking START, the magnetic field is set to the value corresponding to the analysis first species.
- Move the magnetic field thumbwheel of the dedicated keyboard, while monitoring either the bargraph if *EM* or *FC1* or *FC2* was selected, either the MCP image if *SLIT* was selected. (It is not relevant to select *IMAGE*)
- When the B field is correctly tuned (generally, maximum signal on the bargraph), he must click *VALID* in the *Mass Calibration* main window. This current B field value is then transferred into the *Mass Calibration* [m, b] table
- The field is then automatically switched to the next species B field value

5.3.4 Semi auto mass calibration

5.3.4.1 Overview

This Mass Calibration name is labelled "semi-auto" because, on one hand, the B field scanning is launched automatically, and the routine provides with automatic peak centering, but on the other hand, it requires an operator action for validating the peak centering.

The monocollection case

When Clicking onto *PUNCTUAL CALIBRATION*, 2 additional windows are opened:
- The graphic window which diplays the S(B) plot
- The output table window

The multicollection case

The same graphics window as in the monocollection mode is opened, but several curves are displayed simultaneously.

Contents ↑

5.3.4.2 The Semi-Auto *MASS CALIBRATION* panels-1: The main window

The next *Analysis Mass Calibration panel* is opened when clicking *CALIB* from the analysis *SPECIES TABLE* box (See the above section § *The SPECIES TABLE box*.

In the semi-auto mode, the main **analysis mass calibration panel** is identical to the manual mode (See the above section § *The Analysis MASS CALIBRATION panel*).

Contents ↑

5.3.4.3 The Semi-Auto *MASS CALIBRATION* panels-2: The graphic window

This panel is opened when clicking *MASS CAL.SEMI-AUTO* in the *Analysis Mass Calibration panel*
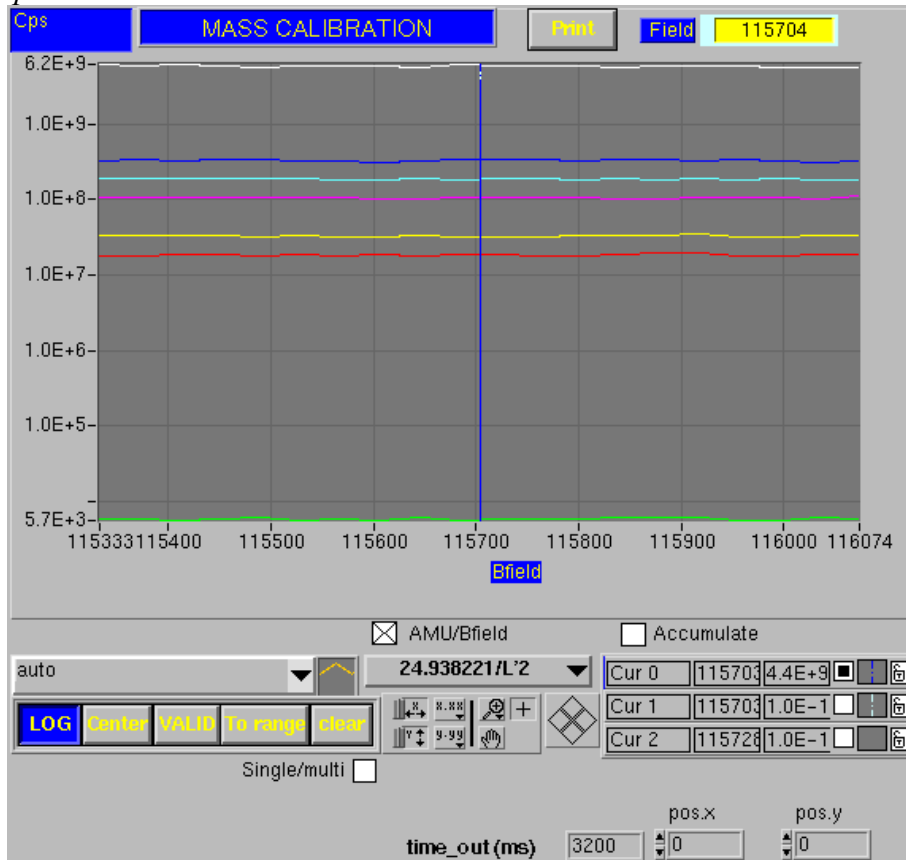
Once this graphic windows is opened, the analysis species table is cycled, and for every field step, the B field is scanned according to the scan parameters defined above in the *main mass calibration window*. With the multicollection mode, there may be several channels involved in a given steps and therefore as many curves displayed at the same time

Auto/ L'2/... allows to select the displayed field step. *Auto* displays in real time the step which is being scanned. Selecting another field step allows to freeze an already scanned peak it if it is necessary to keep it longer in order to centre it manually or automatically.

24.938221/L'2 allows to select the detector which will be used for centering the Bfield.

Single/Multi   To be used only with *Center trolley* Q27

LOG/LIN Switches the Y-axis scale.

Center firstly computes the peak center with the following routine
The y-maximum over all the scan points is detected.
The x-coordinate of the first point at the left hand side such as $y < Ymax/2$ is detected
The x-coordinate $x1$ of the left hand side point corresponding to y1 = Ymax/2 is computed by linear interpolation
The x-coordinate of the first point at the right hand side such as $y < Ymax/2$ is detected
The x-coordinate $x2$ of the right hand side point corresponding to y1 = Ymax/2 is computed by linear interpolation

The peak center is computed as *(x1+x2)/2*

VALID transfers the current mass m *cursor 2* position b to the mass calibration [m, b] table

to range allows to centre the B scan onto the cursor2. If only a part of the peak appears in the graphics window, move the cursor2 towards the peak and click *to range*. Nothing will be changed in the [m, b] table, but the peak will be contained within the B scan.

Clear set the accumulated curve Y(B) at zero. The previous scans are lost.

amu/Bfield Switches the X-axis scale.

accumulate if the box is checked, the successive scans corresponding to the same species are accumulated.

Plot1/Plot2.... allows to select the displayed mass scan, and the to move the cursor and to perform a *VALID*

The *cursor1* corresponds to the value *b* of the mass calibration *[m, b] table*.
The *cursor2*, which can be mouse driven or automatically shifted with *Center* corresponds to the next value of *b* is *VALID* is clicked.
The *cursor3*, corresponds to the value of the *analysis mass* to be analysed, if a *reference mass* is selected for the calibration instead of the *analysis mass*. See below, section § *Reference mass and analysis mass*
WARNING: At the beginning of a mass calibration process, both cursors 1 and 2 are at the same location, at the center of the graphics window.

Contents ↑

5.3.4.4 The Semi-Auto *MASS CALIBRATION* panels-3: The mass calibration table

	CALIB ?	DONE		Mass Symbol	Mass a.m.u.	REFERENCE Mass Symbol	REF.Mass a.m.u.	Detector	Waiting Time (sec)	Counting time (sec)	Offset (V)	Resolution	B Field	Ref Bfield	Trolley position	RMN	B Field RMN
0	YES			28Si	27.9769		0.0000	L'2	0.5	0.50	0.0	300	0	0	0		0
1	YES				0.0000		0.0000	L2	0.5	0.50	0.0	300	0	0	0		0
2	YES				0.0000		0.0000	L1	0.5	0.50	0.0	300	0	0	0		0
3	YES				0.0000		0.0000	C	0.5	0.50	0.0	300	0	0	0		0
4	YES			29Si	28.9765		0.0000	EM	0.5	0.50	0.0	300	0	0	0		0
5	YES				0.0000		0.0000	H1	0.5	0.50	0.0	300	0	0	0		0
6	YES				0.0000		0.0000	H2	0.5	0.50	0.0	300	0	0	0		0
7	YES			30Si	29.9738		0.0000	H'2	0.5	0.50	0.0	300	0	0	0		0

Clear all REFERENCES: CLEAR   Scan Reference Masses only or All : Scaning All

Subscript Number of the species

CALIB (YES/NO) Normally, all the masses must be set to YES. If NO, the calibration will be not proposed for this mass.

DONE   A cross is displayed in the square when the mass is validated. Can be de-validated by clicking the cross.

Mass Symbol, *Mass (amu)* to be considered just as a label for the mass calibration routine.

REFERENCE (Symbol), `EDIT Field`. When this field is filled, at this cycle step, the reference mass will be scanned around during the mass calibration. the analysis mass B field will be computed as

$$B_{ana} = B_{ref} * (1 + 2 * (M_{ana}-M_{ref})/M_{ref})$$

A *reference mass* is to be used whenever the analysis mass signal is to low to be correctly calibrated. Another mass, not too distant from the analysis mass and then called *reference mass* is used for peak centering.

Note that the *reference Mass* can be another specie of the analysis species table. This mau be particularly useful and convenient for *rare earth* analysis where it is difficult to observe any peak for some masses. See also some lines below the selection *Scan Reference Masses only/ Scan all* .

If a *Reference Mass* has been selected for several masses to be analyzed, a single validation is sufficient for all the set of masses defined with this *Reference Mass*.

REFERENCE (amu), `DISPLAY Field`.

Detector, Waiting Time, Counting Time, Offset, Resolution, `DISPLAY Field`. The species table data are displayed there.

Bfield The values of the magnetic field b contained in the mass calibration [m, b] table. Initialized by the analysis species table. Clicking VALID in the graphic window modifies the validated mass.

Trolley position The trolley position for the corresponding species

Scan Reference Masses only/ Scan all If the field *reference Mass* is filled for some masses, this selection allows the operator to check firstly if the peaks can be used for validation. It is then recommended to select *Scan all*. The operator may validate the larger peaks peaks. In a second step, the operator will select *Scan Reference Masses only*, and the program will scan only the reference masses.

5.3.4.5 The semi-auto mass calibration process

Some cycles may be run with the analysis timing for reaching the hysteresis steady state. (Click *CYCLING*, program the *number of cycles*, and click *START* at the window top)

Clicking *START* , at the window bottom menu double bar starts the process. The [m, b] table is filled with the analysis species table data.
- The B field is scanned around the first species mass m_1, and the curve Y(B) is displayed within the graphic window.
- When the first scan is over, the B field is switched to the beginning of the second scan. After the waiting time defined in the analysis species table, the scan around the mass m2 is achieved.
- Once one scan was performed around each mass, the B field is switched again at the beginning of the m_1 scan. A new scan is accumulated to the previous accumulated curve

Y(B), providing that the scan parameters are not modified. If they were modified, the accumulated curve would be automatically set to zero.

So, at any time, it is possible to display within the graphic window a given accumulated curve.

5.4 Running an analysis

5.4.1 Running a single analysis

5.4.1.1 Overview

It is possible to open directly the analysis panels by clicking *ACQUIRE* in the main menu bar. The current *Analysis Definition* file is displayed in the top third field.

It is also possible to open these panels from the main *ANALYSIS SPECIES TABLE* box when clicking *GO TO ACQUISITION*.

In the main *Analysis Control* panel, the set of buttons *START*, *STOP*, *PAUSE*, *CONTINUE*, *ABORT* allows to launch an analysis with different options for stopping it.

Additionally to the main *Analysis Control* panel, either a *curve* window or a *spreadsheet* window is opened. It is possible to switch from one to the other one by clicking *SPREADSHEET*, in the *curve* window or *CURVE* in the *spreadsheet* window. These both windows display the analysis output data in real time, either a "mass versus time" plot for every mass in the *curve* window, or processed into ratios in the *spreadsheet* window. From both the *curve* and the *spreadsheet* windows, it is possible to call post-processing routines. (See the section § *Processing the results with the isotope spreadsheet* in the user's manual (2) or above, the section § *Featuring a High Resolution Spectrum with the "Peak Processing"*

The Isotope analysis output files are saved with the extension .ais

The more current way of running analyses consists of keeping the same analysis definition during a given session and of running it several times on different location. It is also possible to edit this process recipe including the X-Y stage location where the analysis must be run, and to run automatically all this analysis set. See below the section § *Chained Analysis*.
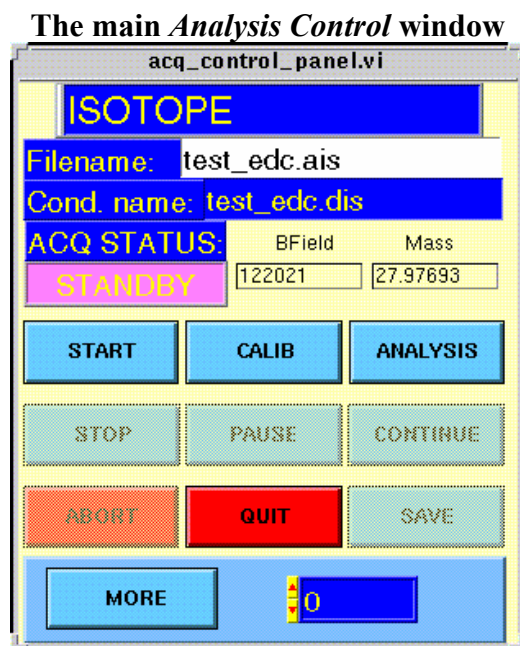

Once an analysis has been started, the analysis B field cycling is going onand can be stopped by only 3 ways:

1. Calling the Tuning
2. Clicking STOP in the Mass Calibration panel
3. Modifying the analysis definition and clicking CALIBRATE or APPLY (The modified cycle is then going on.

5.4.1.2 The main *Analysis Control* panel

The main *Analysis Control* window

ISOTOPE `DISPLAY Field` displays the analysis type (*ISOTOPE/ Parameter/ HIGH RESOLUTION...*)

Filename `EDIT Field` Name of the analysis output file. Default name is the the name of the *Analysis Definition* with a different suffix. When launching successive analyses with the same *Analysis Definition*, the output name is automatically incremented *filename@n*, *filename@n+1*, providing the operator does nor select "*Overwrite*" at the end of an analysis.

Cond name data `DISPLAY Field` Name of the analysis definition file. To download another *analysis definition* file, click *ANALYSIS* for opening the main *Analysis Definition* panel

ACQ STATUS `DISPLAY Field` displays *STANDBY* if no analysis is running and *RUNNING* if an analysis is running.

Bfield `DISPLAY Field` displays the actual Bfield along the cycling.

Mass `DISPLAY Field` displays the species table Mass along the cycling.

START starts the analysis. The analysis cycle will be kept on until it will be stopped by only 3 possible ways:
- Calling the Tuning
- Clicking *STOP* in the Mass Calibration panel
- Modifying the analysis definition and clicking *CALIBRATE* or *APPLY* (The modified cycle is then going on.)

CALIB Calls the *Mass Calibration* routine. In the *Mass Calibration* panel, clicking *APPLY* will recall the *Analysis Control* panel.

ANALYSIS opens the current analysis *Species Table* panel. It allows to modify the analysis definition.

STOP will stop the analysis process at the end of the current cycle. The analysis output file is automatically saved.

PAUSE will stop the analysis process at the end of the current cycle. It allows to modify the instrument settings with the dedicated keyboard. *CONTINUE* will resume the analysis.

CONTINUE must be clicked for restarting an analysis after a *PAUSE*.

ABORT will stop the analysis process at the end of the current cycle. The Analysis output file cannot be saved.

QUIT quits the main Analysis Control panel, but the cycling is still going on.

SAVE saves an analysis output file. To be used for saving partial results in the case of a long analysis, or to save the output file after clicking *ABORT*. Not useful in the general case, since at the end of an analysis, the program propose to the operator either to save the output data in a new file, or to overwrite the previous one.

5.4.1.3 Other windows attached with the Analysis Control

Other windows are normally opened during or after an analysis:
- The curve_browser box
- The curve graphic window
- The isotope spreadsheet

For a description of all of these windows, see below the sub-sections of § *Displaying and processing the Isotope analysis results*.

5.4.1.4 The analysis process

The operator has edited an *Analysis Definition* file and clicked *CALIBRATE*. The *Mass Calibration* has been achieved, all the analysis masses have been validated, and the operator has clicked *APPLY* in the *Mass Calibration* window and *APPLY* in the main *Analysis Definition* window. The *Analysis Control* panel is then opened. The analysis is ready to start.

Before starting the analysis, the operator can select the real time display mode for the analysis results: *SPREADSHEET* or *CURVE*. The last used window (*Spreadsheet* or *Curve*) will have been opened automatically with the main *Analysis Control* panel. In the *Curve* panel, a button *SPREADSHEET* allows to swich to the *Spreadsheet* window, and in the *Spreadsheet* window, a button *CURVES* allows to switch to the *Curve* window.

For an *Isotope* analysis, the operator may select the *Curve* display mode for visualizing the signal stability or the *Spreadsheet* mode for checking at real time the computed ratio relevancy.

Before starting the analysis, it is also recommended to check the analysis filename. The operator is allowed to edit a suitable filename.

The operator clicks START for launching the analysis. The analysis will last upto the defined last cycle if the operator does not click *STOP, ABORT* or *PAUSE*. The operator may click

PAUSE, for modifying the keyboard tuning, and click *CONTINUE* when being back again in the *Analysis Control* Panel.

WARNING: if the operator achieves a mass calibration between *PAUSE* and *CONTINUE*, the mass calibration output will not be taken into account.

During the analysis process, it is possible to switch between both *Spreadsheet* and *Curve* display mode and to modify these both window parameters.

If a Sample HV Control is scheduled during the analysis, when the control occurs, the Sample HV curve in progress is displayed a window specially opened.

At the end of analysis, the program propose by default to save the analysis as *previous_filename@n+1* or to overwrite *previous_filename@n*.

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5.4.1.5 The auto-centering panel

Whenever an automatic control is included within an analysis (*Mass calibration*/ HV Sample/ *Beam Centering*), a control panel is opened in real time when the centering routine is being run.
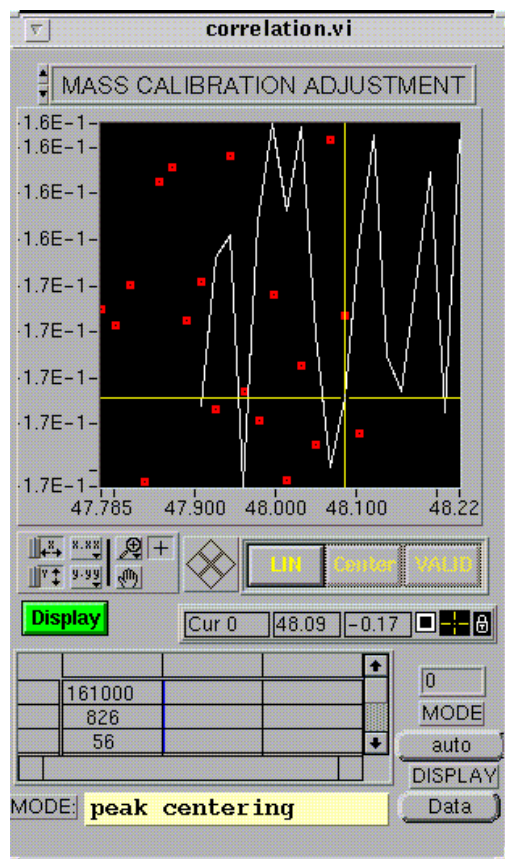
This panel is basically targetted for display. Nevertheless, it is also possible to select the *LIN/LOG* display mode.

It is also possible to select *manual* instead of *auto*. In the manual case, the operator is given the priority. Then he may center the cursor manually or by clicking *center*. The operator gives the priority back to the analysis by clicking *VALID*.

5.4.2 Running chained analyses

5.4.2.1 Overview

The *chained analysis* program allows to run in a batch mode several analyses on different locations of the same sample holder. It is possible to include modifications of any keyboard parameters in the batch, providing that these modifications were recorded and saved in a keyboard file before starting the chained analysis.

The elementary step of a chained analysis is defined by one *(X, Y) position*, one *analysis definition* and *keyboard filename*. The keyboard filename is required only if some keyboard parameters are required to be modified along the chained analysis process. These data are contained in a *Chained analysis definition* file which must be edited previously to the run.

Typical procedure for running chained analyses

- Edit the definition of analyses which must be run in the chained analysis. (*ANALYSIS DEFINITION*)
- Prepare the sample(s) on the sample holder. (Manual operation)
- Open the *CIPS HOLDER* panel.
- Click *LOAD HOLDER* to move the stage to the loading position.
- Load the sample holder into the analysis chamber. (Manual operation)
- Set the instrument in the conditions of the first analysis.
- Prepare step by step the chained analysis process
  - o Move the stage close to the step analysis position (*HOLDER*) while viewing the sample with the optical microscope.
  - o Adust the primary beam and the secondary signal. If some parameters must be modified for this step analysis, record them in a keyboard file (*primary* or *secondary* or *motor* which will be recalled before the analysis.
  - o Record the stage (X, Y) in the Holder list. (*HOLDER*)
- Edit the chained analysis definition with the help of the Holder List. (*Chain Definition*)
- Start the chained analysis. (*Apply* in the *Chain definition* panel + *Start*)

Typical keyboard parameters wich may be modified for an analysis :

- *(v_xpos, v_ypos)* Beam position or *(v_defatx, v_defaty)* Dynamic Transfer for recentering the beam in the *Field Aperture*, in the case of a height sample change. If the Beam Pos must be modified, a *.PRI* file must be recorded and loaded. If *(v_defatx, v_defaty)* must be modified, a *.SEC* file must be recorded and loaded.
- Overall set of primary parameters, in the case of different spot sizes required by different chained analyses (*.PRI* file)
- Entrance slit position (centered over the beam). Then, the *MOTOR* file must be recorded and loaded.

It must be pointed out that the centering routines which have been included in this CIPS 4.0 (See the sections § *The Scan parameter panel* and § *The isotope analysis options (8): Beam Centering* will be preferred to loading new keyboard files.

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5.4.2.2 The chained analysis definition panel

Click *CHAIN* in the main menu Bar, and the following panel is displayed

file (Edit New Chain/ load/ save/ save as) Allows to edit a new chained acquisition or to load a previouly defined chained acquisition or to save the present edited chained definition. *load, save* ans *save as* opens a dialog box (See below *the chained analysis file dialog box*).

Item `Display Field` will be automatically incremented (buttons *Insert item*, *delete item* and *clear table* may also be used)

X:Y `Editing Field` Clicking on this field opens a box purposed to select a point in a *Holder List* (See the section § *The stage Navigator (Holder)*in the user's manual (2). Select the point and click *OK* in the *Holder list* panel. X and Y can also be edited manually.

Analytical Condition file `Editing Field` Clicking on this field opens a box purposed to select an *Analysis Definition* file. (See above the section § *Defining an isotope analysis*). In the first line, this field is required to be filled. In the following lines, this field is not required to be filled. In this case, when a new line will be validated with a new name, all the empty lines will be filled by the *Analysis Definition* filename of the last defined line.

Destination file `Editing Field` is the name of the data output file. If this field is not filled, it will be automatically incremented.

Acquisition time, `Display Field`, computed according to the analysis definition data

VALID (Yes/No) if *No*, this line analysis will not be run.

Keyboard conditions `Editing Field` Clicking on this field opens a box purposed to select a Kbd file which will be loaded just before the analysis. These files are normally located in the directory *Cipsdata/Keyboard*. It is necessary to fill this field only if the Kbd parameters are required to be modified. *Primary*, or *Secondary* or *NEG*, or *Motors* files can be selected. **.GLO* files cannot be loaded.

Insert Item Inserts a new line in the analysis definition at the marked location.

Delete Item Deletes the marked line.

***Clear table*** Clear the chained definition table. It will be ready for a new edition.

PRINT for printing

total acquisition time `Display Field` is the computed overall analysis time

APPLY creates the chained analysis file name and may increment automatically the destination filenames if only the first field is filled. It opens also the *Chain Control* panel (See the next section § *[The chain analysis control panel](#)*)

QUIT for quitting the panel

The chained analysis file dialog box
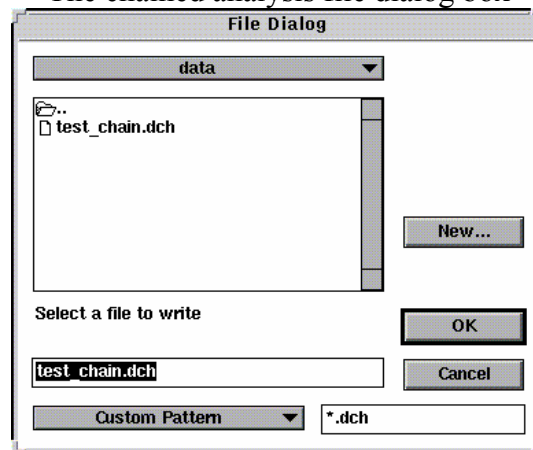
5.4.2.3 The chain analysis control panel

For opening this panel, click *APPLY* in the *Chain Analysis Definition* panel
The chained analysis which is started from this panel must have been defined in the *Chain Analysis Definition* panel.
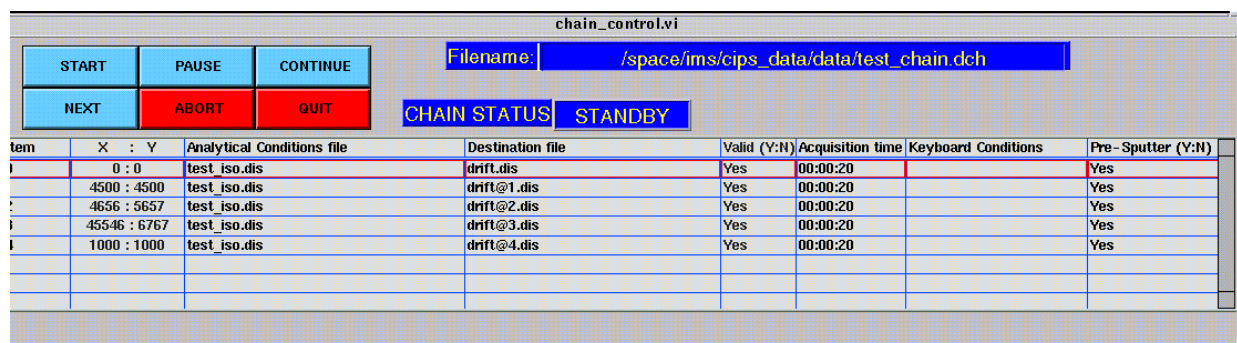
filename `Display Field` the chained analysis filename defined in the *Chain Analysis Definition* panel.

START for starting the chained analysis the filename of which is displayed in the field *filename*. Opens *main Analysis Control* the panel. The first analysis is automatically started.

PAUSE during the *chained analysis* process, it has the same effect as for an analysis. See the section § *The main Analysis Control panel*

CONTINUE After a *PAUSE*, same effect as for an analysis. See the section § *The main Analysis Control panel.*
NEXT After a PAUSE, the analysis in progress is not finished. The next analysis is started.

ABORT Aborts the chained analysis process.

QUIT quits the panel.

CHAIN STATUS Display Field

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6. Other Analysis

6.1 Overview

The Species table

6.2 Depth Profile

DEPTH PROFILE

ANALYSIS TIME: (s) `0.0`

CYCLE NUMBER: `1`

BEAM BLANKING :	☐	
PRE-SPUTTERING	☒	...
REFERENCE SIGNAL	☐	...
MASS CALIB. CONTROL	☐	...
HV SAMPLE CONTROL	☐	...
OVERLAPPING CRATER	☐	...
BEAN CENTERING	☐	...

Contents ↑

6.3 Energy scanning

ENERGY

ANALYSIS TIME: (s) `0`

ENERGY (min): (eV) `0.00`

ENERGY (max): (eV) `0.00`

Number of steps: `0`

SAMPLE ▼

BEAM BLANKING :	☐	
PRE-SPUTTERING	☐	...
REFERENCE SIGNAL	☐	...
BEAN CENTERING	☐	...

6.4 Linescan

6.5 Mass Spectrum

MASS SPECTRUM

ANALYSIS TIME: (s) `30`

WAITING TIME: (Total) (S) `0.10`

#Measurement: `1.00`

#dM: `4`

BEAM BLANKING : ☐
PRE–SPUTTERING ☐ `...`
REFERENCE SIGNAL ☐ `...`

BEAN CENTERING ☐ `...`

COMMONS PARAMETERS

Waiting time (sec)FC `0.00`

Duplicate first line For all Species: set Waiting Time   set Counting Time   set Offset   Compute Waiting time

Symbol	Mass	Symbol (high)	Mass	Detector	waiting (s)	counting (s)	offset	resolution
O	15.9949	Al	26.9815	EM ▼	0.1	0.10	0.00	500
	0.0000		0.0000	EM ▼	0.5	0.50	0.00	0
	0.0000		0.0000	EM ▼	0.5	0.50	0.00	0
	0.0000		0.0000	EM ▼	0.5	0.50	0.00	0
	0.0000		0.0000	EM ▼	0.5	0.50	0.00	0
	0.0000		0.0000	EM ▼	0.5	0.50	0.00	0
	0.0000		0.0000	EM ▼	0.5	0.50	0.00	0
	0.0000		0.0000	EM ▼	0.5	0.50	0.00	0

GO TO ACQUISITION   **CALIB**   **CANCEL**

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7. (Displaying and processing the Isotope analysis results)

See *The IMS 1270 CIPS user's guide (2)*

8. (The EM Control and EM drift correction)

See *The IMS 1270 CIPS user's guide (2)*

9. (The stage Navigator (*HOLDER*))

See *The IMS 1270 CIPS user's guide (2)*

10. (Image Processing)

See *The IMS 1270 CIPS user's guide (2)*

11. (TOOLS)

See *The IMS 1270 CIPS user's guide (2)*

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12. (Appendices)

12.1 (Appendix 1: The EM Physical Principles)

See *The IMS 1270 CIPS user's guide (3)*

12.2 (Appendix 2: The EM drift correction principles)

See *The IMS 1270 CIPS user's guide (3)*

12.3 (Appendix 3: The QSA effect)

See *The IMS 1270 CIPS user's guide (3)*

12.4 (Appendix 4: The Faraday cup Measurement principle)

See *The IMS 1270 CIPS user's guide (3)*

12.5 (Appendix 5: Fundamental of Statistics)

See *The IMS 1270 CIPS user's guide (3)*

12.6 (Appendix 6: LabVIEW® graph options and graph cursors)

See *The IMS 1270 CIPS user's guide (3)*

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