User's Manual for

ANALYST

version 2.00

An IBM-PC Computer Program for Control of a Thermal-Ionization, Single-Collector Mass-Spectrometer

Kenneth R. Ludwig[1]

U. S. Department of the Interior
GEOLOGICAL SURVEY

OPEN-FILE REPORT 92-543

[1]U.S. Geological Survey, P.O. Box 25046, Mail Stop 963, Denver, Colorado 80225

1992

TABLE OF CONTENTS

PREFACE

Analyst is a computer program for controlling an Isomass 54 mass-spectrometer with an IBM-compatible computer. The program combines error-tolerant ease-of-use with a high degree of flexibility and power in acquiring research-quality isotope-ratio data. Optimization routines built into the data-collection modes yield the highest quality isotope-ratio data per unit time, even in the face of varying degrees of ion-beam stability.

The program is designed such that, even when executing complex automated routines, the user can always either interact with the operation of the routines in real time or regain complete manual control within no more than a second. Graphical feedback to the user is provided wherever possible, which, when combined with detailed alphanumeric feedback, informs the user of the status and functionality of the program at any time.

How Should You Use This Guide?

For your first session with *Analyst*, start with the **Manual Running** section. This will give you some familiarity with the way you will interact with *Analyst* and get you to the stage of actually running samples in a fairly short time.

When you're comfortable with doing manual runs and are ready to experiment with fully-automatic runs, use the **Automatic Running** section. You might then try fully-automatic runs of the same samples you had been experimenting with in the manual-running mode.

To access some of the less-frequently used functions of *Analyst*, to deal with non-routine situations, or just to understand more about the capabilities and logic of *Analyst*, you'll eventually want to consult the **Reference** section. The **Reference** section is not particularly coherently arranged, but is better-suited to finding out how to access specific functions of *Analyst* (or to find out if a function is available at all). The **Reference** section contains instructions on how to load *Analyst* from scratch, what to do after loading in a barrel of new samples, and how to define new *Elements*.

If you really want to dig into the nuts and bolts of the program, you may want the program list (on disk). The program contains about 27,000 lines of code, however, and several hundred subprograms, so the program list alone (without the HTBasic environment) is of very limited use. To obtain the program list, with or without the supporting datafiles, write directly to Ken Ludwig at the U.S.G.S. (Mail Stop 963, Denver CO, 80225).

Hardware/Software Required

The particular mass spectrometers for which *Analyst* was written are VG-Micromass Isomass 54E and 54R models, built in 1979-80. These machines are equipped with a single Faraday-cup collector using a 10^{11} ohm resistor, an analog Daly Detector, and a 16-bit GPIO interface. The 54E has a 16-sample motorized barrel, the 54R a 6-sample manually-rotated barrel.

The minimum computer for running *Analyst* is an IBM-PC compatible system with an 80386-33 Mhz CPU, numeric coprocessor, hard disk, VGA color graphics, 4 MB of RAM, 40 MB hard disk, and the TransEra GPIO board. The "joystick" used by *Analyst* is actually an *ICONtroller*[1]. *Analyst* is written in HTBasic 3.3 (TransEra Corp., Provo, Utah), and requires this language/operating system to be running.

---

[1]Suncom Technologies, 6400 W. Gross Point Road, Niles, IL 60648.

Running *Analyst* in Emulation Mode

If there is no mass spectrometer connected to the computer, *Analyst* will automatically simulate responses, so that many of the typical features and actions of the program can be experienced without an actual mass spectrometer attached. The simulated ion beam will be a function of the filament currents (no beam will be present if the simulated filament currents are off). Normally, in emulation mode, all printer output is suppressed. If you want printer output directed either to the printer as usual, or redirected to the screen (results in a somewhat messy display), invoke the ***Emulation Mode Setup*** screen by pressing either **↑F5** from the **↑F6 Hardware** menu, or **Alt E**(mulate) from the *bms*.

The emulator will simulate realistic mass-spectra, ion-beam intensity (as a function of filament current) and ion-beam noise for several common elements (K, Ca, Rb, Sr, Ba, Re, Pb, U, and Th), and so permit reasonably realistic simulated automatic runs. However, because the emulator does not have to wait for the mass-spectrometer to measure an ion-beam, wait for the magnet to slew, the barrel-motor to move, or the Daly-deflection voltage to decay, the emulated mass spectrometer can run many times faster than a real one. If you want more-realistic timing, increase the ***Emulation Mode Time-Delay Factor*** from the ***Emulation Mode Setup*** screen. A value of 1 approximates the speed of a real mass-spectrometer, while smaller values result in progressively faster responses.

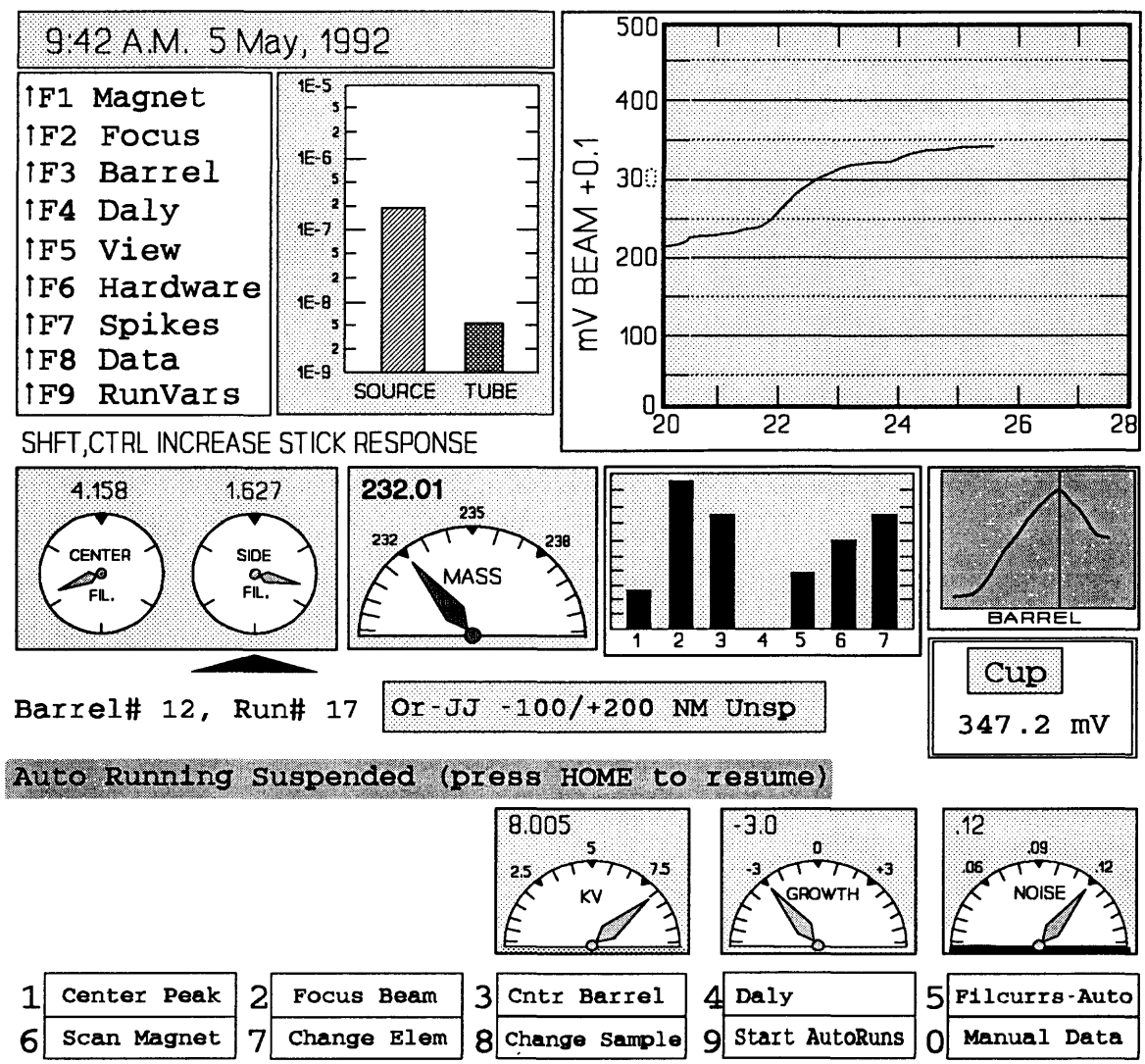
The ***Emulation Mode Setup*** screen also asks:

`Enable update of hardware-status disk-files?`

If the computer you're running will not be connected to the mass spectrometer, answer Yes. But if the computer is the normal mass-spectrometer controller, you should probably answer No, because otherwise files used by *Analyst* to specify the calibration and/or state of the mass spectrometer can become revised by emulated (that is, imaginary) conditions. However, if you're careful to either avoid, or to restore after exiting from emulation mode, any barrel contact-tests and magnet drift-adjusts, as well as revisions of standard run-variables, amplifier time-constants, spikes, elements, default-focus settings, et cetera, you can enable disk-file updates (to provide more complete and realistic emulation) even though the computer is connected to the mass spectrometer.

MANUAL RUNNING

This section is intended to be used while you're sitting down at the computer and actually running a trial sample. To start, you'll need to have a sample in the barrel that you can play with, and have the mass spectrometer pumped down, all switches turned to their proper settings (see p. 78), and the beam valve open. Check with an experienced operator to make sure that this is the case. Ask this person to also make sure that *Analyst* is currently showing the *beam-monitor screen* (*bms*) - in which the ion-beam is being continuously monitored, the filament-currents, focus-positions, and magnet positions shown, and either an explanation of the shifted function-key functions shown at the upper-left of the screen, or the letters *bms* shown at the lower-right of the screen.



The *bms* screen

Interacting with *Analyst*

The Function Keys: -- The function keys are the keys labeled **F1** through **F12** at the top of the keyboard. In many parts of *Analyst* (including the *bms*) what the function-keys do is indicated by labels in highlighted rectangles, with numbers to the left indicating which function-key they represent, at the bottom of the screen.

In many cases, *Analyst* will also explain the functions of the function keys in more detail above the key labels. Whenever you press a function key that has a label, *Analyst* will usually immediately perform the labelled operation (though some require either confirmation or further operator input).

The menus obtained by pressing a *shifted* function-key from the *bms* are shown at the upper-left of the screen. Note that a symbol such as **↑F8** means to hold down the *shift* key when pressing the function-key.

The (joy)Stick: -- *Analyst* is designed to use the ICONtroller joystick as input from the *bms* (and some other contexts) to change the filament currents or magnet position (the cursor-keys can also be used). To increase the response of the joystick, hold down **Shift**, **Ctrl**, or both together (in order of increasing response) while moving the joystick.

Recovering from I/O Errors: -- *Analyst* is protected against most I/O (Input/Output) errors such as a non-responding printer or non-responding parts of the mass spectrometer. For example, if the printer is not turned on or out of paper, a message to that effect will appear on the screen every time the program attempts to use the printer, and the output will be temporarily diverted to the screen. To put things right, just fix the printer problem. If some part of the mass spectrometer is not responding, however, this can be fatal to the run; *Analyst* will display a message indicating the type of problem, and after trying a few times to re-establish communication, will stop all operations. If you find the program in this state, try to fix the problem, then press **Alt F3** to re-start the program.

It is possible, though, for an I/O problem to occur which the program does not trap; in such cases, the computer will simply lock up. If you find the computer in this state, press **Alt F5** to clear the I/O transaction, *write down the line-number that appears after you do this*, then try to fix the problem if you can. Press **Alt F3** to re-start the program.

Starting to Use *Analyst*

First, press **Esc** until the full menu and status information (shifted function-key menus at the upper left, beam-chart at the upper-right, filament-current dials at the middle-left of the screen) is displayed. This is the "top-level" or "home base" of *Analyst*, called the *Beam-Monitor Screen* (*bms* for short). When you're at the *bms*, *Analyst* is waiting for a command from you, while at the same time monitoring the intensity of the ion beam that is arriving at the collector. You'll be returned to the *bms* after completing most operations or if you intervene during automatic running. You can command any operation of *Analyst* from the *bms*, and many of these operations are available only from the *bms*.

On-Line Index to Analyst's Functions: An immediate, on-line guide to the functions provided by *Analyst* from the *bms* is available by pressing the ? (or /) key. Pressing ? from the *bms* gives you immediate access to a complete index of all of *Analyst*'s functions together with the keystroke-combinations required to invoke these functions. Just press the first letter of the function or class of functions that you want to access (for example, press S for the keystroke-index of Spike-related functions). As long as you keep pressing one of the letter-keys, you will access the keystroke-index for that letter. The index (included in this manual, starting on p. 63) is redundant (the same function exists in the index by several names), so you should be able to locate what you want fairly quickly.

Changing Filament Currents

There are three ways of changing filament currents (all from the *bms*)[1]:

1) Press the button on the top of the joystick (or press the asterisk key) to enable keyboard-commanded filament-current change. A large red pointer will flash beneath the filament-current dial (left-center of the *bms* screen) for the active filament (center or side, sample or preheat). Select the filament you want to change with the left/right arrows of the cursor keys. Move the joystick away from you to increase that filament current, or towards you to decrease the current. Increase the response of the joystick by holding down **Ctrl**, **Shift**, or **Ctrl Shift** (in order of increasing response) as you move the joystick. The filament-current dials will continuously update the filament-currents as they are changed.

2) As above, but use the up/down arrows of the cursor keys.

3) Press **F5** to invoke the automatic filament-current change *Form*. The advantages of this method, which will be explained in detail later, are that you can change the currents at a reproducible rate and unattended.

Changing the Magnet-Position

Though there is a flexible, graphical magnet-scan routine for scanning over the local mass-spectrum (**F6** from the *bms*), you can shift the magnet from the *bms* directly, with immediate beam-graphics update, with the following keys:

[1]If you've invoked a "large" beam-chart, or if graphics for some just-completed procedure are being preserved on the screen, the bms will consist only of a single line of information towards the bottom of the screen: the status-dials, focus-bars, and shifted-function key menu will not appear. *Nonetheless, all of the usual bms functions, including the shifted-function key menus, are still invoked with their usual keystrokes.*

Keystroke	Response
+	Jump to peak-top of next mass *up*
-	ditto, to next mass *down*
]	Jump to the high-mass side (to ~half-peak height) of the present peak
[	Ditto, to *low*-mass side
>	Jump to half-mass position (background) just *above* the present peak
<	Ditto, *below* the present peak
Spacebar	Jump to peak-top nearest the present mass
PgDown	Jump *to* the ^{187}Re peak (if defined for the current **Element**)
PgUp	Jump *from* the ^{187}Re peak to a normal peak for the current **Element**)
Alt →	Scan magnet slowly *up* mass (or move joystick to the **right**)
Alt ←	Scan magnet slowly *down* mass (or move joystick to the **left**)
Ctrl F*n*	Jump *up* ***n*** mass-units
Ctrl Alt F*n*	Jump *down* ***n*** mass-units

The mass-dial of the *bms* screen will always show you what mass is currently arriving in the collector.

Other *bms* Dials and Gauges

A bar-gauge at the center-top of the *bms* screen shows the source-can and flight-tube pressure of the mass spectrometer, updated every 10 seconds or so (after the last keystroke). The accuracy of the pressure gauge depends on a calibration done with a pressure-calibration file (see the **↑F6 Hardware** menu to view, create, or add to this file).

The filament-current dials at the left-center of the *bms* screen always show the filament currents of all filaments present for the current sample. There may be 4 dials shown (if you have preheat filament-contacts installed), 2 dials (for a triple-filament sample with no preheats), or only 1 dial (single-filament sample, no preheats).

To the right of the mass dial is bar-gauge showing the settings (0 to 999) of the focus-unit. With experience, the appearance of this gauge will help you recognize badly aberrant focus-positions at a glance. The eighth bar of the gauge is present only for triple-filament samples, and reflects the center-side filament potential.

Once you have an ion-beam for a sample and have invoked the barrel-centering routine by pressing **F2**, a small graph at the right-center of the screen shows the response of the ion-beam to a short-range scan of the barrel. The vertical line in this graph indicates the present position of the barrel. Barrel-scan graph trends that are very short indicate a sample that will lose filament-contact if the barrel is moved very much.

Towards the right-center of the screen, a double-lined box indicates the current collector (Faraday cup or Daly detector), and the ion beam currently arriving in that collector, in millivolts. Assuming a 10^{11} ohm resistor, a 1-millivolt ion-beam is equivalent to about 62,000 ions per second, or an ion current of 10^{-14} amperes.

At the bottom-center of the screen is a dial showing the accelerating voltage (high voltage) set on the focus panel of the instrument. The accelerating voltage dial is updated every 15 seconds or so; if a significant change is detected, the accelerating voltage will be continuously queried for the next 5 seconds, on the assumption that you are changing the setting from the focus-panel, and would like to know the resulting change in KV.

If you have a relatively large ion-beam (greater than about 100 mV for the Faraday cup, or about 30 mV for the Daly), you can invoke ion-beam noise and growth dials at the bottom-right of the *bms* screen by pressing **F12**. These dials reflect the integrated behavior of the ion-beam over the last several seconds, and may be useful in evaluating beam stability. The beam-growth units are percent change per minute, and the beam-noise units are percent change per second. If the computer has a fast CPU (a 33-MHz 80486 or faster), the beam growth/noise dials will be invoked automatically when the *bms* is invoked if the existing ion beam is >1 volt (Cup) or 30 mV (Daly).

Manipulating the *bms* Beam-Chart

A graphics box showing the ion-beam intensity is present by default at the upper-right corner of the *bms* screen. You can re-scale this chart in a variety of ways with simple keystrokes from the *bms*. Re-scaling functions available are:

L Toggle between a large chart (occupying most of the screen) and a small chart (in the upper-right corner of the screen). The large-chart *bms* screen condenses the filament-current, mass, magnet, and ion-beam intensity information to a single line, but *all of the* bms *keystroke-invoked functions remain active.*

G Toggle between a chart with a Linear ion-beam scale and a chart with a loGarithmic ion-beam scale. The latter is especially useful as you are bringing up a filament-current to obtain an ion-beam for the first time.

X Toggle through 3 levels of increasingly expanded ion-beam scales, back to un-expanded. The third level of expansion is scaled to the collector in use and the size of the ion beam, such that the theoretically-limiting noise of the beam occupies about 5% of the chart-height.

U/D Increase/decrease the "headroom" (amount of Y-space above the current beam-size) of a linear-scaled beam-chart.

Shift U/D Increase/decrease the time shown by the X-axis of the beam-chart.

F11 Re-scale the chart to fit the size of ion-beam presently being collected (using the currently-specified headroom or expanded scale).

Access to Other Functions of *Analyst*

The simplest (but not fastest) way of invoking other *Analyst* functions is to select the general category of the function you want from the shifted function-key menu at the upper-left of the *bms* screen:

↑F1 Magnet
↑F2 Focus
↑F3 Barrel
↑F4 Daly
↑F5 View
↑F6 Hardware
↑F7 Spikes
↑F8 Data
↑F9 RunVars

Pressing any of these *shifted* function-keys from the *bms* gives a menu to a variety of related functions (all of the menus are shown on pages 71-74). For example, the Magnet menu (**Shift F1**) allows you to determine peak flats, abundance-sensitivity, adjust the magnet calibration for peaks, et cetera. Many of the shifted function-key functions can also be accessed by shortcut keys, which are shown in brackets at the right of the shifted function-key menus. Thus you can request a magnet drift-adjust either by pressing **Shift F1**, then **F10**, or by simply pressing **M**, the shortcut-key.

Storing and Retrieving Screen Files from *Analyst*

You can store any screen-image from the *bms* by pressing **Ctrl Enter**, then entering any legal DOS filename. Usually, you won't want to specify a disk or path for the file, as the default SCREENS directory (from which the screen files can be easily accessed from *Analyst*) is the most useful. For example, after the Magnet Scan routine (**F6** from the *bms*) is finished, the graphics for the scan will remain on the screen after you are returned to the (one-line) *bms*. To store that screen for later retrieval or printer-dumps, simply press **Ctrl Enter** as indicated above.

To retrieve a screen file, press **Enter** from the *bms*. Select the screen file from the list-box, examine the resulting image on the screen, and dump the image to the printer if you like. Note that the first files in the list-box all have the **.ANL** extension. These are screen files automatically saved by *Analyst*, and include displays for the last:

Abndsens.Anl ..... Scan for abundance-sensitivity/resolution
Autoscan.Anl ..... Within-run auto-run diagnostics scan
Contacts.Anl ..... Filament-contact scan (current sample)
Hallscan.Anl ..... Hall-Probe troubleshooting scan
Hvdrift.Anl ..... High-voltage drift test
Lastaver.Anl ..... Weighted averages
Lastcont.Anl ..... Filament-contact scan for barrel
Lastscan.Anl ..... *bms*-invoked magnet scan
Pkflat.Anl ..... Quantitative peak-flat graphics
Pkshape.Anl ..... Quick peak-shape scan
Pressure.Anl ..... Pressure versus time graph
Timecons.Anl ..... Time-constant calibration graphics
Zero.Anl ..... Collector zeroes

If you no longer need a screen file, delete it (put the list-box cursor on the file and press **Delete**) to avoid filling the computer's hard disk.

Some Other Common (non-Function) keystroke-functions from the *bms*

- To turn a filament **off** *immediately* (as opposed to turning the filament off by a continuous decrease of current), press the **1, 2, 3,** or **4** key *twice* within a half-second interval. This will turn off the center or side filament in the *running* position (**1** or **2**), or the center or side filament in the *preheat* position (**3** or **4**). To turn *all* filaments off at once, press the **5** key twice.

- To re-draw the *bms* screen, press **Esc**.

- To dump *any* screen to the printer, at almost any point in the program, press **Ctrl PrintScreen.**

- To invoke a complete beam tune-up (peak-center, focus, barrel-center, focus again), press the **Tab** key.

Exiting from Commands or Operations

If you accidentally invoke a function, or simply want to terminate some operation, pressing the **Esc** key will usually back you out in a graceful way. Other ways of stopping the program and re-entering running are:

- In an emergency, press **Ctrl Pause.** This will crash the program and return you to the HTBasic operating system (indicated by the word "Reset" at the lower-right of the screen). To re-start the program and return to the *bms*, either (1) press **Alt F3**, or (2) clear the screen by pressing the **Home** or **End** keys, type the word **RUN** and press the **Enter** (or **Return**) key.

- If the program appears "hung up", it may be due to a hardware I/O problem. Try pressing **Alt F5**; if a program line then appears at the bottom of the screen, the problem was indeed with the interface. Press **Alt F3** to restart, and note the occurrence in the log-book so this hardware problem can be fixed later.

- If *Analyst* is doing an automatic run and the **F1** key is defined as **→Manual**, press **F1** to return (within a second or two) to the *bms*, where you will have full control. You can return to automatic running (at about the point where the automatic run was interrupted) from the *bms* by pressing either **Home** or **←Backspace.**

Exiting from *Analyst*

If you just want to temporarily exit to DOS and perform a few simple operations (such as file or disk management), press **F8 DOS Shell** from the *View* menu (**Shift F5** from the *bms*) - or simply press **Ctrl End** from the *bms*. The SHELL function will allow you 64 kilobytes while in DOS. To return to *Analyst* from DOS, type EXIT and press **Enter**.

To completely exit to DOS, press **F8 Quit** from the *View* menu (**Shift F5** from the *bms*). If any of the filament currents are on, *Analyst* will ask you whether you want them turned off. The complete state of the program

will be saved to disk before you exit, so that if you return to *Analyst* within a couple of hours, you won't have to go through the whole start-up procedure, which includes resetting the barrel.

Getting a Beam (Manual Running)

To experiment with *Analyst* any further, you'll need to obtain an ion beam from your sample. First, using the + or - keys, jump to the most abundant isotope in your sample. Then, increase the center and (if a triple-filament sample) side filament currents until you have a significant ion-beam (preferably at least several millivolts). Center the magnet on the peak by pressing **F1 Center Peak.**

Now press **F2 Focus.** The beam-focus operation adjusts the potentials on each of the source plates to maximize the ion-beam intensity. Several (automatic) iterations of adjustment are usually required, and may take up to a minute or two for the first focus of a sample. The graphics plot at the left of the focus screen shows how the ion-beam changes with each focus-step, while the plot at the right of the focus-screen is a graph of the ion-beam versus the settings of the different "plates" of the ion-beam collimator.

When the beam is focused, press **F3 Center Barrel.** The barrel-center routine rotates the barrel slightly to obtain maximum beam-intensity. The graphics will show you how sensitive the beam size is to the barrel position.

You should now have a centered and focused ion beam. To get more intensity, increase the sample-filament current until you have a useful beam size. Incidentally, you can duplicate the complete tune-up sequence described above (once you have some sort of ion beam) by just pressing the **Tab** from the *bms*. *Analyst* will then center the peak, focus the ion optics, optimize the barrel, and focus again, without any additional commands.

Switching Collectors -- Faraday Cup and Daly Detector

The Daly Detector permits a large amplification of the ion beam with almost no amplification of signal noise, as well as almost completely eliminating background noise. The limitations of the device are that:

1) The intensity of the ion beam arriving at the Daly must be no more that about 50 millivolts to avoid damage to the Daly;

2) The gain of the Daly varies slightly with the mass of the arriving nuclide, resulting in a near-linear mass-discrimination in the range of 0.1% - 0.4% per mass-unit;

3) There can be a significant nonlinearity in the response of the Daly as a function of the intensity of the arriving ion-beam, so this nonlinearity must be calibrated for really accurate data. I have observed a value of about 0.35% over the 50 mV range of the Daly, such that at a 50 mV beam, the gain of the Daly detector was about 0.35% less than for much smaller beams. Within error, the non-linearity appeared to be linear with beam size.

The latter two points are discussed more fully later (see pages 21 and 58), but for now just regard the Daly as a device which greatly increases the signal-to-noise ratio of an ion beam. If you're worried that you could inadvertently damage the Daly Detector by accidentally exposing it to a very-intense beam, you needn't be. The Daly is extensively protected against such damage both by *Analyst* and, for most models of the mass spectrometer, by the Daly hardware itself.

To toggle between the Faraday Cup and Daly Detector, press **F6** while in the *bms*. If you're switching to the Daly and the nuclide arriving at the collector wasn't previously "cleared" at the present filament-current for use with the Daly, *Analyst* will quickly check to make sure that the beam is not too intense before switching on the Daly. If you look at the beam-chart, you may notice a slight change in the apparent beam-size when you change to the Daly Detector, and a marked reduction in the beam noise. If the beam-size discrepancy between the Faraday Cup and Daly Detector is more than about 20 percent, you may want to recalibrate the Daly gain (**Shift F4, F3** or just **Alt D** from the *bms*).

Reaction of the *bms* to Large Beams

Analyst won't tolerate an ion beam that is too intense for the collector in use. The maximum acceptable beam for the Faraday cup is 10 volts (10^{-10} amperes), and the maximum acceptable beam for the Daly Detector is about 50 millivolts (5×10^{-13} amperes). If a beam of more than 10 volts arrives at the Faraday cup, *Analyst* will immediately switch to either the next-higher or next-lower isotope with an acceptable beam-size. If a beam of greater than 10 volts is obtained while *not* in the *bms* (for example, while focusing), *Analyst* will reduce the sample-filament current until an acceptable beam is obtained.

If the Daly Detector is in use when an unacceptably large beam is obtained, *Analyst* will immediately switch to the Faraday Cup. Should this occur, there will be a 6 second delay before the beam can be detected in the Faraday Cup.

Using *Analyst*'s *Form* Screens

Some operations can't be initiated with just a keystroke-command or two; several items of information might be required first. For such operations, *Analyst* will present you with a *Form* to fill out and submit. If you've filled out the *Form* with no errors or misunderstanding, *Analyst* will proceed with the specified task as specified by the *Form*. For example, try the semi-automatic method for changing filament currents. Press **F5 FilCurrs-Auto** from the *bms*. A *Form* will appear on the screen, looking something like this:

```
Filament to change                        1
(1=center-sample   2=side-sample,
 3=center-preheat, 4=side-preheat)

New Current (amperes) --------------> ??
 (present CF=1.234, SF=0)

Rate of Change (milliamps/second)         10

Show Beam-Graphics (Y/N)?                 No

Beam-Target in mV (0 if none)             None
Beam-Target Isotope                       "
Beam-Target Abort-Current (amps)          "

ENTER each value, CTRL-ENTER or F12 when done  (ALT-R = Recall)
```

Notice that one of the values on the right (probably the **New Current** value) is shown highlighted and with a dashed arrow pointing to it. This is the value that the *Form* is requesting you to type in. You can move the "parameter cursor" to any parameter (row) you want with the Up/Down arrow keys, the joystick, or Home/End (=Top/Bottom of *Form*). To enter a value, just type it in when the parameter-cursor is where you want it. *Note that nothing you type in will be retained unless you press the ENTER key* -- if you move the parameter cursor without ENTERing the value, your entry will disappear.

Notice that when the *Form* appears on the screen, some of the parameters will already have reasonable default-responses, but other parameters will have a double question-mark. The double question-mark indicates a parameter that *must* be filled in. For many *Forms*, you can get more detailed explanations of what the parameters are and how to fill in the form by pressing the **HELP** function-key (**F1**). When you do so, the screen will show you information for either the whole *Form*, or for the current *Form* parameter.

As long as you have the semi-automatic filament-current *Form* on the screen, I'll discuss its use here. The upper-most parameter of the *Form* indicates which filament will have its current changed; 1 for the *center* filament of the sample in *running* position, 2 for the *side* filaments of the sample in *running* position, 3 for the *center* filament of the sample in the *preheat* position (that is, the sample whose barrel-number is one greater than the sample in running position), 4 for the *side* filament in the *preheat* position. The **New Current** is just the current that you want the filament taken to, in amperes.

The **Rate of Change** refers to how rapidly you want the **New Current** to be attained. For example, if you choose a **Rate** of 10, the filament current will be changed at a nominal rate of about 10 milliamperes per second. So to go from 1.0 to 2.0 amperes will take roughly (2-1)*1000/10/60 = 1.7 minutes. If you are increasing a filament current by a large amount, *Analyst* will check the source pressure every several tenths of an ampere, and if the pressure is too high, will wait until it goes down before increasing the filament current again. You can turn this option off if you like, during the filament-current take-up.

Your response to the **Show Beam-Graphics?** parameter determines whether *Analyst* will show real-time beam graphics at the same time as the filament-current change. If you want to see what the ion beam is doing while the filament current is changing, enter **Y**(es).

The last three parameters of the *Form* are used only if you want *Analyst* to automatically obtain a certain beam-size after having taken the filament to the **New Current** value. To do so, specify the **Beam Target**, the **Beam-Target Isotope**, and the **Beam-target Abort-Current**. The **Beam Target** is the beam size that you want, *in millivolts*, with a tolerance of 10%. The **Beam-Target Isotope** is isotope which must give this beam size. The **Beam-Target Abort-Current** is the maximum sample-filament current (in amperes) that *Analyst* is allowed to use to obtain the **Beam Target**.

Complete the *Form* and submit it to *Analyst* by pressing the **Ctrl Enter** or **F12**. The screen will then show the filament currents as they change, and also allow you to change the rate of change at any point in the process. To alter the take-up or take-down rate of the filament current, press either the **Double Rate** or **Halve Rate** function-keys: the rate will immediately change in response. If you want to abort the process, just press **Esc** immediately return to the *bms*.

Scanning the Magnet

To scan the magnet (with graphics), press **F6 Scan Magnet** from the *bms*. The resulting *Form* will look something like this:

```
Start scan at mass ----------------> 203.5
End scan at mass                     209.5
Scan speed (mass-units/second)        .2
Use Daly or Cup

Linear or Log Scan (Lin/LoG)         LIN
Max. Beam on graph (mV)              10000

Single scan (1), Repeat one direc-
 tion only (2), Repeat Up/Down (3)   1

Use Dump colors (Y/N)?               N
Line (1) or Solid (2) beam-trace     1

Coarse-magnet range (0-10)           8

Hall probe check
(troubleshooting only)               No

ENTER each value, CTRL-ENTER or F12 when done   (ALT-R = Recall)
```

In the above example, the scan would start at mass 203.5 and make one scan up-mass to 209.5 at a nominal rate of 0.2 mass-units per second. Useful values for the scan speed are typically between .05 (very slow scan) to 1 (very fast scan). You can speed up or slow down the scan as it is being done, though, so don't worry about the exact value. You can scan either up-mass or down-mass. If you specify a repeated scan, the routine will continue to repeat the scan (using a different pen-color each time) until you press **Esc**.

The **Max. beam on graph** parameter indicates the Y-axis height for the graphics. Generally, you'll want a value about 20% greater than the size of the largest peak that will be included in the scan. You can choose either a linear or logarithmic Y-axis, depending on what you enter for the **Linear or Log scan** parameter. Logarithmic scans are extremely useful if the scan will encounter peaks of very different sizes. Enter **LIN** (or just **L**) for a linear Y-axis, **LOG** (or simply **G**) for a logarithmic Y-axis.

The scan will start with whichever collector you specify in the *Form* (Daly or Cup). If you specified the Daly and a peak of more than 50 mV is encountered during the scan, *Analyst* will quickly switch to the Faraday Cup, then back again to the Daly as soon as the beam-size permits. This feature is very useful if you want to look at the fine details of the mass-spectrum, so don't hesitate to specify the Daly even though there will be large peaks in the scan.

The **Coarse-Magnet Range** parameter refers to which of the 10 coarse-magnet ranges the magnet is set to, with the default range being the one appropriate for the current *Element*. For example, if the current *Element* were Pb, and you wanted to see if any potassium peaks were present, you would either change the **Coarse-Magnet Range** to the appropriate lower value, or temporarily change the *Element* to potassium or calcium. When you submit the **Scan Magnet** *Form* with some other coarse-range value, the *Form* will re-appear and ask you to define the starting and ending *magnet values* instead of the starting and ending *isotopes*. These magnet values can range from 0 to 9999.

The **Use Dump Colors?** query allows you to specify whether the screen will show the beam-trace and axis labels on a black background (= "Dump Colors") or a white background. The latter color scheme cannot be dumped to the printer, as both the beam-trace and the background will appear black.

With the **Solid (1) or Line (2) Scan**, you can specify scan-graphics with a line indicating the trace of the scan over the peaks (1), or with the peaks completely filled in (2).

The **Hall Probe Check** parameter is used only for trouble-shooting. A response of **YES** to this parameter gives a scan with the Hall-Probe Output (proportional to the magnetic field) as the Y-axis rather than the beam size. This type of scan should *always* give a smooth, nearly linear trace, within the noise of the Hall-Probe Output and the 1-pixel resolution of the screen. If the Hall Probe is malfunctioning, *Analyst* will detect the problem and point out the location of the suspect output on the scan-graphics.

Changing *Elements*

An *Element* is a set of data that tells *Analyst* what element you're running, what nuclides can be present, what nuclide to use as the default reference-isotope for isotope ratios, what isobaric interferences to expect and how to correct for them, if fractionation-normalization is possible and what ratios and values to normalize to, and where to take backgrounds for data-taking. The most common *Elements*, such as Pb, Sr, U, Nd... have probably already been defined using conventional constants for isobaric interferences and fractionation-normalization. When you get more familiar with *Analyst*, you can easily define a new *Element* of your own (pages 48-53), or perhaps define another version of an existing *Element* (for example, if you wanted to normalize Nd runs to the 148/144 ratio instead of the 146/144 ratio).

Try changing the *Element* that you're now using to another one -- say Nd. Press **F7 Change Elem.** from the *bms*. The screen will then show you a list of *Elements* that have been defined and stored on the disk. Choose the **Nd** *Element* by pressing the **N** key until the cursor-bar is on **Nd**, and press **Enter**. *Analyst* will retrieve the information for running neodymium from the disk and display a screen similar to the following:

```
ELEMENT Nd        Last modified by KRL on 11:28:19     4 Nov 1992
 Ba134      Ba135      Ba136      Ba137      Ba138      La139
 Ce140      Pr141      Nd(Ce)142  Nd143      Nd(Sm)144  Nd145
 Nd146      Sm147      Nd(Sm)148  Sm149      Nd(Sm)150  Eu151
 Sm152      Eu153      Sm154      Gd155      Gd/Dy156   Gd157

 Reference Peak: 144
 Normalizing Ratio:  144/146=1.38523
 Report Ratios as: i/144                      HV for Element: 8000
 Daly Mass-Discrim: 0.29%/a.m.u.
 Data-Taking Backgrounds Above & Below Each Peak

    Monitor Isotope        Interferes with          Ratio
         147                    144              144/147=.2097
         147                    148              148/147=.7478
         147                    150              150/147=.4957
         140                    142              142/140=.1251
```

The first several lines of the display show which nuclides have been defined for this *Element*. Though you can move to any local mass-position from any *Element*, you can only take isotope-ratio data for those nuclides which are defined for the *Element*. If none of the existing *Elements* include the isotopes you want (or if none of them has the fractionation-normalization and isobaric-interference corrections they way you want), you'll have to edit the *Element* or define a new one (see the **Reference** section).

The **Reference Peak** isotope is important only if the *Element* can be normalized for fractionation; that is, it contains two isotopes whose natural ratio can be considered to be invariant, so that any mass-fractionation occurring during the process of analysis can be corrected for by normalizing to an assumed value for this ratio. Examples of such elements are strontium, neodymium, hafnium, and calcium. For fractionation-normalizable *Elements*, the **Reference Peak** is one of these two isotopes and is also the isotope to which all others will be ratioed for isotope-ratio determinations. For example, if the **Reference Peak** is 144, then the data will be calculated as either **i**/144 or 144/**i**, where **i** is any other isotope. Whether 144 appears in the numerator or the denominator of the ratios was the choice of the person who defined the *Element*.

The accelerating voltage (**HV**) that must be present for the magnet-settings of the nuclides to be valid is indicated by **HV for Element: 8000**, above. If the accelerating voltage differs by more than 3 volts from the indicated value, *Analyst* will continue to query until either the accelerating voltage is close to the *Element*'s value, or you press **Esc**. Note that *Analyst* looks at the *digital* value of the accelerating voltage, *not* the setting on the instrument panel. To find out what the present digital HV value is, press **Ctrl V** from the *bms*.

The **Normalizing Ratio (144/146=1.38523** in the above example) is the isotope ratio that will be used for fractionation normalization. If such a ratio exists, than *all* blocks of data for this *Element* <u>must</u> contain this ratio as well as the ratio of interest.

The next line down (**Data-Taking Backgrounds Above & Below Each Peak**) indicates that the data-taking backgrounds will be taken about a half-mass (or less, if the nuclide mass is less than about 140; at mass 86 the offset is about 0.3 mass-units) and below each peak. This is the most-common method, though you can specify that backgrounds be taken at a single mass-position for more-rapid (but less accurate in some cases) data acquisition.

The next lines indicate what isobaric interferences may be present and how to correct for them. In the example, *Analyst* will know that there may be interferences at masses 144, 148, 150, and 142, and that they can be corrected by monitoring masses 147, 147, 147, and 140, respectively. The corrections will be made by subtracting .2097, .7478. and .4957, respectively, of the 147 peak, and by subtracting .1251 of the 140 peak. These numbers, of course, refer to the ratios of naturally-occurring Sm, Sm, Sm, and Ce, respectively.

In *Analyst*, unlike most commercial software, the information in the *Element* files is separate from the information on how to do automatic runs. *Analyst* is designed this way because *Elements* need to be defined only rarely, and having to do so again with each new automatic run is a nuisance. And also, the separate *Element* files permit the operator to run in the "manual" mode with a minimum of set-up information.

Looking at the Rhenium Beam

You can switch the magnet to the ^{187}Re peak for most *Elements* (if they were defined at a center-filament current of more that about 4.4 amperes) by pressing **PageDown** from the *bms*. You may need to center the Re peak the first time that you do this for a particular sample. To switch back to the peaks of the *Element* you're running, press **PageUp**. A rhenium beam should be present whenever a center rhenium filament is hotter than about 1850°C.

Changing Samples

To change samples (that is, to rotate another filament-assembly into running position), press **F8 Change Sample** from the *bms*. *Analyst* will display a list of the samples, together with the currently-defined sample names, and the number of filaments as determined from the last barrel contact-test. Move the cursor bar to the sample you want, and press **Enter**.

NOTE: If the number of filaments in the list is invalid, you must correct the discrepancy by pressing ***F1 Change Fils****. You can then over-ride the default value for that filament. If you do not do this, unpredictable responses to filament-flag checks may result.*

When you've selected a sample, *Analyst* will reset the barrel (rotate it to its reset position just below barrel# 1), rotate to the approximate position of the sample you specified, find the interval of barrel rotation where good filament-contacts exist, and determine the backlash of the mechanical assembly for this sample. The backlash should be in the range of 3 to 15 -- values outside this range generally reflect either contact problems or barrel-drive problems. The interval of good contacts would be at least 15 units; if less, the screen will display a warning message indicating possible contact problems. If the screen tells you that no filament-contacts were obtained, check that the knobs on the filament power-supply on the mass spectrometer are really on by turning them to the **RESET** position, then back to **ON**.

After rotating the new sample into position, *Analyst* may take a minute (if more than an hour has elapsed since the last zero-determination) to determine the collector zeroes and noise. Finally, before returning to the *bms*, *Analyst* will reinstate the default focus-settings for the current *Element* from disk.

Taking Isotope-Ratio Data Manually

Once you have a beam large enough for data-taking, you can ask *Analyst* to take as little or as much data as you want, while still controlling (if you want) beam-size and beam-growth. Though I will refer to this mode of data taking as "manual", in fact it is a semi-automatic mode that lacks only the capability for obtaining a proper beam to start with, and for automatically changing samples.

To start manual data-taking, press **F10 Manual Data** from the *bms*. If the *Element* that you're using is one that *will* be normalized for mass-dependent fractionation using an internal isotope ratio (such as Sr or Nd), the first *Form* to appear will look like this:

```
Data-Taking, Spiked Samples

Sample Name -------------------------> ??

Spike Number (0 if unspiked,
 press F4 to select from list)          0

Normalize data to ratios of
 first block (Y/N)?                     No
```

The **Sample Name** is just the name that you assign to this run of this sample. It can be up to 50 characters long, so you can be fairly descriptive.

The **Spike Number** tells *Analyst* if this sample has been spiked, and if so, which spike. Spiked runs will be discussed later (p. 25), but for now just note that you can store the isotope ratios of a spike for a fractionation-normalizable (or double-spikeable) element. *Analyst* can then calculate both the ratio of the sample isotopes to the spike isotopes, and also a radiogenic-isotope ratio corrected for both fractionation and contamination by spike isotopes. The simplest way to specify a spike for manual data-taking is to press **F4** and select from the list of defined spikes. If you need to change the **Spike Number** later (in the middle of the run), you can do so by invoking the ***Spikes*** menu from the *bms*. Instructions on creating a new **Spike** are given on page 55.

The **Normalize Ratios to First Block?** parameter asks whether, instead of using the usual (natural) ratios for fractionation-normalization, you'd rather use the appropriate normalizing ratio of the *first block*. For example, suppose that you want to determine the ratios for a new ^{150}Nd spike, and your usual normalizing ratio for Nd runs is 146/144=.7219. The new spike, however, might have 146/144= 3.456, in which case using .7219 would give very strange results.

But if you choose to normalize all of the other ratios of the run to whatever 146/144 ratio you get for the first block, the normalized ratios will not be too far from the true values. The main advantage here is that because all of the blocks will have been normalized for a fractionation relative to the first block, you can perform a weighted averages on the ratios for all of the blocks and then correct the *averaged* ratios for whatever true fractionation you predict. *Any averaging procedure on fractionation-uncorrected blocks with consistent ratio-drift makes no sense.*

The next *Form* (or the first one, if the *Element* is not fractionation-normalizable, such as Pb, Rb, Lu...) will look something like this:

```
                    Define Data-Taking Blocks

 Sample Name -------------------------> ??

 Isotopes (reference isotope first)     238,235

 Number of Sets in a block              15
 Number of Blocks                       1

 Beam Window (most-intense peak):
  Minimum Beam (volts)                  0
  Maximum Beam (volts)                  10
  Maximum Filament-Current (amps)       6

 Maximum Beam-Growth (%/minute)         100

 Final Filament-Currents (amps)
 (sa-Cen,sa-Si,preh-Cen,preh-Si)        4.128,2,234,0,0,0

 Daly Status (0,1,2)
 (0: Disabled   1: OK for data
  2: Beam-tuneup only)                  1

 Integration/delay times specified
  by Analyst or Operator?               A

ENTER each value, CTRL-ENTER or F12 when done    (ALT-R = Recall)
```

Notice that at most, only the sample-name query *must* be answered (that is, the default response is ??). So when this *Form* appears for the first time, it's already almost completely filled out with default responses. As a general rule, if you're not sure of a response to a query in this (or any other) *Form*, accept the default responses -- they will give you a simple but adequate mode of data-taking.

The Isotopes Query for an *Element* without Internally-Normalized Fractionation: -- Enter a list of the isotopes for which you want isotope-ratio data, separated by commas. You must enter the reference isotope *first* in the list; the order of the remaining isotopes is irrelevant. For example, if you wanted 206/208 and 206/207 ratios, your response would be either

206,207,208

or

206,208,207

Any isotope that is defined for the *Element* can be chosen as the reference isotope.

Don't include isotopes whose only purpose is to monitor for isobaric interferences, such as ^{85}Rb for strontium runs or ^{147}Sm for neodymium runs. These isotopes will be automatically monitored if necessary.

The Isotopes Query for an *Element* with Internally-Normalized Fractionation: -- For an element such as Sr, where the ^{86}Sr/^{88}Sr ratio is used to normalize for mass-dependent fractionation, the **Isotopes** query will look like this:

```
Isotopes (must include 86 and 88)?
```

In other words, no matter what other isotopes you wish to include, you *must* include the two isotopes (86 and 88 in the above example) that will be used for fractionation-normalization.

If on the previous *Form* you specified that the sample were spiked, another isotope would be required. For example, for Sr runs, the resulting query would be:

```
Isotopes (must include 86, 88, and 84)
```

If *none* of the data-taking isotopes have a peak greater than about .02 millivolts, *Analyst* won't be able to center any of the peaks and will refuse to take data. But if there is at least one significant-size peak present in the local mass-spectrum, you can specify this peak as the *Centering Isotope* by entering it in either square brackets or parentheses after the data-taking isotopes. The *Centering Isotope* need not be present in your list of data-taking isotopes (though it must exist in the *Element*'s list of isotopes).

For example, to take data for ^{229}Th and ^{230}Th, but to use ^{232}Th to estimate the magnet-positions for the ^{229}Th and ^{230}Th peaks, the **Isotopes** response would be **229,230[232]**. The centered ^{232}Th peak magnet-position would then be used to estimate the ^{229}Th and ^{230}Th peak-positions, no attempt would be made to center the 229 and 230 peaks, and only 229/230 data would be taken.

Note, however, that if you specify a *Centering Isotope*, any specified Beam Window parameters then pertain to the *Centering Isotope* peak, not, as usual, to the most-intense peak.

The Number of Sets in a Block and Number of Blocks Queries: -- A *set* is defined as a single sequence of peak-top jumps during data-taking. For example, if the isotopes were 206, 207, and 208, a set would consist of the peak-jumping sequence over all three isotopes. A *block* of data consists of a complete sequence of peak-top jumps during data dating, including peak-centering, backgrounds, monitoring for isobaric interferences, and ratio calculation.

Typical *blocks* consist of 10 to 30 *sets*. The greater the number of *sets*, the longer it will take to do a *block* and the more precise the data in the *block*. Except for ^{206}Pb-^{207}Pb-^{208}Pb-^{204}Pb, the peaks are centered only at the beginning of each block, so choose the number of sets to give a block of no more than about 15 minutes in length. The number of sets you specify may be increased somewhat by *Analyst* if (1) the previous block of this run were also for the specified isotope ratios, (2) the previous block's precision showed that the ion beam was unstable. In this case, the integration times and delay times for the peaks will be shortened from the stable-beam values.

The Beam Window Queries: -- After each block, *Analyst* checks to see if the intensity of the Most-Intense Peak (**MIP** for short) or Centering Isotope (see above) lies within the **Minimum Beam** and **Maximum Beam** limits. If the beam lies outside this "window", *Analyst* will raise or lower the sample-filament[1] current until the **MIP** (or Centering Isotope) lies within the specified beam-window. Note that the default values -- 0 and 10 -- are equivalent to specifying that no limits be placed on the beam size.

The **Maximum Filament-Current** parameter puts a limit on how high the sample-filament current can be taken to satisfy the **Minimum Beam** requirement. For example, if the **MIP** (or Centering Isotope) fell below the **Minimum Beam** and the **Maximum Filament-Current** were 2.42 amps, *Analyst* would not increase the filament current past 2.42 amps even though the **Minimum Beam** were not attained.

If your sample is on a triple-filament assembly with a rhenium center-filament, you can also specify a window for the ^{187}Re beam-size. To do this, add a slash after each of the beam-window values that pertain to the **MIP**, then add the ^{187}Re specifications. For example, if you wanted to specify a beam window for the most-abundant uranium isotope of between 0.6 and 1.2 volts with a maximum side filament-current of 3.5 amps, together with a beam-window for ^{187}Re of between 0.2 and 0.25 volts and a maximum center-filament current of 5.5 amps, your entries for the **Minimum Beam**, **Maximum Beam**, and **Maximum Filament-Current** parameters would be **.6/.2**, **1.2/.25**, and **3.5/5.5**, respectively.

The Growth-Limit Query: -- This parameter restricts how fast *Analyst* will allow the ion-beam to grow during data-taking. If the beam is growing too rapidly, *Analyst* will reduce the sample-filament current by 2.3 percent.

The default **Growth Limit** value of 100% is equivalent to placing no constraints on beam growth. This is appropriate for many types of runs, including those for Pb or U. For elements such as Sr, Nd, and Th, however, rapid growth generally indicates that the ion-beam will soon go into a rapid and irreversible decline. In such cases, reducing the sample-filament current within a few minutes of the onset of such growth can usually salvage the run. **Growth Limit** values in the range of 2.0 to 3.5 percent per minute seem to be appropriate for these types of runs.

[1]The sample filament is the filament that the sample is actually loaded on -- center if a single-filament assembly, sides if a triple-filament assembly.

Usually, too-rapid growth will cause *Analyst* to turn down the filament current only *after* a block is completed. However, if the growth-rate is extremely high -- more than *twice* your specified limit -- *Analyst* will exit the block in the middle of data-taking and immediately turn down the filament(s)[1].

The Final Filament-Currents (amps) Query: -- After completion of the blocks specified in the **Number of Blocks** query, *Analyst* will change any or all of the four possible filaments to the values specified in the **Final Filament-Currents** parameter. The response to the query is in the from of 1 to 4 values, separated by commas, such as **1.85,3.0,1.62**, or **3.0,1.62,2.5,1.8**. The order of the values corresponds to the filaments that they affect, such that:

First value	→	center filament,	running position
Second value	→	side filament,	running position
Third value	→	center filament,	preheat position
Fourth value	→	side filament,	preheat position

The default values that will always appear in the *Form* are simply the filament currents that were in effect when the *Form* was invoked. In other words, if you make no entries for the **Final Filament-Currents** parameter, no action will be taken at the end of the specified number of blocks.

One additional function you can specify with *Final Filament-Currents* is that, after all of the specified data-blocks are done, weighted averages will be calculated and printed out for all relevant ratios. To request this option, add the letters **AV**(erage) after any *Final Filament-Current* specifications (for example, **3.0,1.62 AV**). If you don't want any changes in the filament-currents after the last block but do want the weighted averages, just enter **AV**. Of course, you can request the weighted averages routine from the *bms* for any run (p. 31).

The Daly Status (0,1,2) Query: -- This parameter specifies the conditions under which the Daly Detector can be used. The significance of the possible responses (0, 1, or 2) is:

0: Specifies that the Daly is either malfunctioning or not installed, and must not be invoked at any time under any conditions. *Don't enter 0 unless the Daly is actually missing or malfunctioning.*

1: Specifies that the Daly can be used with appropriately small beams (<50 millivolts or so) for *both* beam tune-up *and* for data-taking. Beam tune-up includes centering, focusing, and barrel-adjust. For the Daly Detector to be used for data-taking, *all* of the data-taking isotopes must be <50 millivolts.

2: Specifies that the Daly *can* be used when necessary for beam tune-up, but *cannot* be used under any circumstances for data-taking (even if all of the peaks are small).

[1]Should this happen more that 3 times in a run, however, *Analyst* will assume that the problem is an unstable or spiking beam rather than simple too-rapid growth. In such a case, *Analyst* will no longer monitor for excess beam-growth during data-taking for the rest of the run.

The advantage of the Daly Detector is that the background noise is reduced to almost nothing (the equivalent of about 10 ions per second), and the peak-top noise is reduced to that of ion-counting statistics. Thus the internal precision of a block of data taken with the Daly is generally immensely improved compared to Faraday Cup precision.

The disadvantage of the Daly is that it introduces both a pseudolinear mass-dependent bias in favor of the lighter isotope, and also a nonlinearity (so the Daly gain varies slightly with the size of the ion beam). So if you want to get results with the Daly at an accuracy level of 0.1-0.2%, you'll need to calibrate the Daly for both nonlinearity (p. 58) and for mass discrimination. You'll have to calibrate the mass discrimination factor, probably for each *Element*. The best way is probably to just bracket a Daly block with two Faraday Cup blocks for the isotopes of interest. You can then store the calculated mass-discrimination factor with the *Element*, so that isotope-ratio data will be automatically corrected for this bias. If this brief explanation isn't adequate, then you probably shouldn't be doing the calibration yourself.

The Integration/delay times Query: -- Normally, *Analyst* will calculate the optimum times for peak-top integration and delay-times before integration begins. For the first data-block, these times are based on a stable beam, and will yield the most precise data in the least amount of time. If the beam becomes unstable, *Analyst* will automatically shorten both the integration and delay times, to better track the beam's instability. Enter the letter **A** for this (default) option.

In some cases, however (perhaps precise data isn't needed), you may want to specify the integration and delay times yourself. If so, enter the letter **O**. After you submit the *Form* with **F12** or **Ctrl Enter**, *Analyst* will ask you to specify the integration and delay times for each data-dating peak; for example:

```
Operator-Specified Integration & Delay Times

Integration, Delay times (secs) for 233 ---> 4,2
    "          "     "     "     "  234      4,2
    "          "     "     "     "  235      4,2
    "          "     "     "     "  236      4,2

(Enter Analyst for auto-calculated times)
```

Keep in mind that *Analyst*'s peak-jumping sequence for data-taking is always from the largest to smallest peak, in order of decreasing peak-size. The time required for the magnet to switch peaks is only 1 second for small mass-jumps (less than about 1 part in 80, and increases to about 3 seconds for jumps greater than about 1 part in 20. Note also that background times will increase/decrease proportional to the peak-top integration times.

If you want to specify integration/delay times for just *some* of the peaks, enter **A**(nalyst) for those peaks whose integration/delay times *Analyst* is to be left to calculate. For example, if you were taking ^{206}Pb-^{207}Pb-^{208}Pb-^{204}Pb data, but you wanted only minimal time spent on the ^{208}Pb peak, you might enter **1,1** for the 208 times, and **A** for the others. *Analyst* would then be able to optimize the integration/delay times for the ^{206}Pb-^{207}Pb-^{204}Pb peaks according to the beam's size and stability, while still minimizing the time spent on the ^{208}Pb peak.

HELP Screens for the Manual Data-Taking *Form*: -- Many of *Analyst*'s *Forms* have HELP screens available by pressing **F1**. These HELP screens may pertain either to the whole *Form*, or only to the parameter the *Form* cursor is on. Press **Esc** to return to the *Form* after reading the HELP screen.

The Data-Taking Procedure

Data taking begins as soon as you submit the manual data-taking *Form* to *Analyst*. First, *Analyst* checks to see if you've forgotten to focus the ion beam. If so, the beam will be focused at this point. Then, all of the specified peaks will be centered, and quick step-scan over each data-taking isotope performed so that *Analyst* can know the approximate intensities for each isotope. From the step-scan information, *Analyst* will select:

1) the order of peak-switching during data-taking (always from most-intense peak to least-intense peak),

2) Unless operator-specified (p. 21), the delay times before integration for each peak (the greater the ratio of the previous peak to the present peak, the greater the delay time; also, increased delay times may be selected for large magnet-jumps),

3) Unless operator-specified, the integration times for each peak (the smaller the peak, the larger the integration time),

4) the amount of time spent on backgrounds, and

5) Unless specified with the *Element*, the mass positions where backgrounds are taken.

For a stable ion-beam, *Analyst*'s choices will give the highest precision of the isotope ratios in the least amount of time, and will minimize the corrections for the resistor time-constants. The algorithm is based on the equations given in Ludwig (1986).

However, if the previous-block's data (for the same isotopes) exhibited significant excess variance, *Analyst* will (unless over-ridden by operator-specified integration/delay times for *all* peaks) modify the stable-beam algorithm such that:

1) the integration and background times will be shortened and made more equal for the different peaks,

2) the delay times will tend to be shortened, and

3) the number of sets will be increased so that the elapsed time for the block will remain roughly the same.

These modifications will allow any beam-instability to be "tracked" more effectively, permitting significantly greater precision than if the "stable-beam" integration and delay times were used. If the beam becomes more stable during the run, the integration/delay times will increase again towards their optimum values.

Basic Data-Taking: No Isobaric Interferences or Fractionation Correction

In its simplest mode (isotopes with neither isobaric interferences nor fractionation normalization; not a ^{206}Pb-^{207}Pb-^{208}Pb-^{204}Pb block), data-taking proceeds as follows:

1) The source-can and flight-tube pressures are checked. If either pressure is greater than permitted by the specifications in the Hardware Configuration file (**Shift F6 F8** or **H** from the *bms* to access), a warning message is printed out. For automatic runs, *Analyst* will wait up to 30 minutes for the pressure to improve, then abort the run if the pressure is still too high.

2) Backgrounds (zeroes) are taken[1]. If a) the flight-tube pressure is less than 2.5×10^{-9} and the source-can pressure less than 4×10^{-8}, b) the largest ratio of the data-taking isotopes is less than 20 (less than 5 if fractionation-normalized and unspiked or with a radiogenic-isotope ratio), and c) the Faraday Cup is the collector, then backgrounds will be measured above and below the least-intense peak only. If these conditions are not all met, or if the calculated best-offset is less than ½ mass-unit, then backgrounds will be taken above and below *all* of the peaks. The amount of background offset is set at the lesser of ½ mass-units or 0.34% of the mass.

   Background readings are filtered for noise spikes and (Faraday Cup only) checked for consistency with the known dark-noise of the collector. If the backgrounds are anomalously noisy, the background readings at that position will be repeated once. Background integration times are optimized for the size of each peak, with some additional time added for Daly-detector data under high flight-tube pressure conditions.

3) Peak-top switching and integration begin. Real-time graphics of the beam are shown on the screen (p. 26), as well as real-time ratios and the approximate 2σ variation (in percent) of the set-data *(note that these ratios are used for display purposes only, and are corrected neither for isobaric interferences nor spike isotopes)*. Peak-top data for small peaks on the Daly detector are filtered for spikes with a biweight algorithm. *Analyst* will note any apparent beam-dropouts, and will exit the block immediately in the case of extremely intense beams (>10 volts for the Faraday cup or >50 millivolts for the Daly) and in the case of beam-growth that exceeds twice the assigned **Growth Limit** value.

4) Backgrounds are taken again, in the same sequence as the backgrounds taken before the peak-switching.

5) Final isotope ratios are calculated and results printed out.

6) The isotope ratios, precisions, filament-currents, and time at the mid-point of the block since the start of the run (the time when the sample was rotated into running position) are stored on disk.

7) If the intensity of the most-intense peak lies outside the beam window specified in the manual data-taking *Form*, the sample-filament current is raised or lowered to adjust the beam size.

---

[1]Unless the previous block of data were for the same isotopes and at the same filament-current. In this case, the previous block's after-peaktop backgrounds will be used as the current block's before-peaktop backgrounds. Peaktop-jumping can then begin as soon as the block starts.

8) If the average growth-rate of the beam during the block exceeded the limit specified in the manual data-taking *Form*, the sample-filament current is reduced.

Data-Taking with Isobaric Interferences

If isobaric interferences can be present (remember, monitor isotopes for isobaric interferences should *not* have been specified as data-taking isotopes in the manual data-taking *Form*), the data-taking procedure is modified as follows:

1) Backgrounds are taken above and below each monitor isotope (a monitor isotope is one that is used to estimate the intensity of an interfering peak; for example, mass 85 (=^{85}Rb) to indicate ^{87}Rb interfering with ^{87}Sr for strontium runs).

2) Before starting peak-top switching, the monitor peaks are measured for 10 to 30 seconds (optimized for the specific run).

4) If the amount of interference as calculated from any of the monitor peaks is *greater* than 0.1% of the isotope that is being interfered with, that monitor isotope is added by *Analyst* to the list of isotopes for peaktop-switching.

5) If the calculated amount of interference is *less* than 0.1%, the peak will be monitored again only after the peaktop-switching sequence.

6) Correction for isobaric interferences is made from either a least-squares cubic interpolation of the monitor peaks (case 4, above), or from a linear interpolation of the monitor peaks (case 5, above).

7) Variances due to isobaric-interference corrections are included in the calculation of the final uncertainties of the ratios. *These variances include an arbitrary uncertainty of 2% in the assumed (interfering peak)/(monitor peak) ratio, to reflect the fact that the degree of mass-fractionation of the isotopes of the interfering elements is poorly controlled.*

Data-Taking for ^{206}Pb-^{207}Pb-^{208}Pb-^{204}Pb Blocks

Because ^{204}Pb is always a minor isotope for natural Pb (and almost all spiked Pb), and because Pb-isotope ratios relative to 204 are critical for geochemical studies, blocks of Pb-isotope data involving all four natural isotopes of Pb[1] are taken in the following manner:

1) a first series of 206/204 ratios is taken, with the number of sets being about 2/3 of the number specified in the data-taking *Form*;

2) the 206 peak is centered and any magnet-drift corrected;

3) a block of 206/207/208 ratios is taken, using the number of sets specified in the data-taking *Form*;

[1]The block must also have 206 specified as the reference isotope, in the numerator of the reported ratios, for this method to be assumed by *Analyst*.

4) the 206 peak is again centered to correct for any magnet drift;

5) a second series of 206/204 ratios is taken with the same number of sets as the first series;

6) statistics for the two 206/204 series are combined to give a single set of statistics for the 206/204 ratio.

This sequence of peaktop-switching gives extra time on the critical 204 peak, retains short interpolation times for the major 206, 207, and 208 peaks, and cancels out any fractionation drift for the 206/204 ratios compared to the 206/207/208 ratios. Though such blocks can take rather a long time (20 minutes or so for a specified 15-set block), the fact that any magnet-drift is corrected twice during the block makes the procedure quite reliable.

If you *don't* want Analyst to take ^{206}Pb-^{207}Pb-^{208}Pb-^{204}Pb data in this way, either:

1) add the # symbol after your list of specified data-taking isotopes (manual data-taking only),
2) specify an isotope other than 206 as the reference peak,
3) add or subtract to the 206,206,208,204 isotope list for the block's data,
4) use operator-specified integration/delay times (see p. 21).

For data-blocks that include 206/204 and 206/207 ratios and with 206/204 ratios greater than 100, *Analyst* will calculate and print out the approximate radiogenic-^{207}Pb/^{206}Pb age for each block. This calculation assumes a .12%/a.m.u. mass-discrimination and a Stacey-Kramers initial-Pb composition.

Data Taking with Fractionation Normalization

If the *Element* is one that has two isotopes whose ratio can be used for normalization of mass-dependent fraction, such as Sr and Nd, then a linear regression of that isotope ratio during the time of the peaktop switching will be used to correct for mass fractionation. Thus the fractionation can change significantly during the block without increasing the uncertainty of the corrected ratio(s). The added variance arising from this correction is included in the calculation of the uncertainties of the corrected ratios. The fractionation law used is the exponential law discussed by Russell and others (1978).

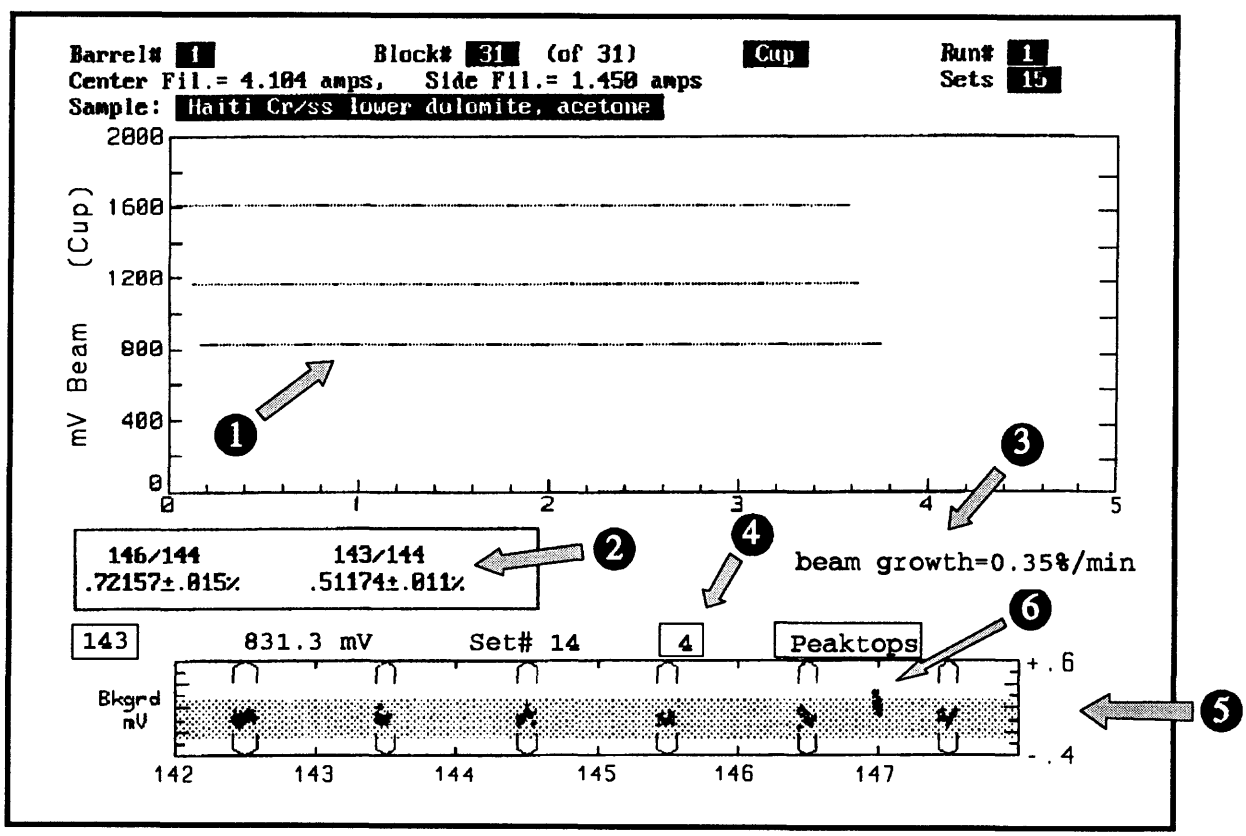
Data-Taking for Spiked Runs

For runs of either fractionation-normalizable elements with an added spike isotope, or of other elements with an added double spike (such as ^{233}U+^{236}U-spiked uranium), the run will be treated as an *un*-normalized element until after all the isotope-ratio data has been obtained and printed out. At this point, *Analyst* will calculate the ratio of the sample's *reference* isotope to the spike's *most-abundant isotope* (this ratio is called **SAM/SPK** by *Analyst*). Like the data-reduction for unspiked-runs, this calculation uses an exponential fractionation-law (Russell and others, 1978).

If a ratio for a radiogenic isotope were also measured, the ratio of the radiogenic isotope to the reference isotope will be corrected for both spike isotopes and fractionation, and the corrected ratio indicated by an asterisk rather than a slash (for example, **87*86** rather than **87/86**). The errors propagated by the fractionation-correction and the spike-isotope subtraction are also calculated, and are included in the reported **SAM/SPK** and radiogenic-isotope ratios.

The Data-Block Screen

During data-taking block, *Analyst* displays a lot of information about the progress of the block, so that you can evaluate beam-stability, real-time ratios, and background readings.



The Data-Block Screen

Key features of the data-block screen, indicated by numbered arrows in the example above are:

❶ Beam-traces for each nuclide, solid for the time during which the beam for that nuclide is actually measured, dotted for interpolations. Each nuclide is shown with a different color. The X-axis scale of the beam-trace box is in minutes.

❷ Real-time median ratios (in the same color as the beam-trace of the non-reference isotope), with 2σ uncertainties of the *sets* (not of the mean of the sets; therefore the uncertainty of the block mean will always be less). Real-time ratios are corrected for fractionation (unless the run is both spiked and fractionation-normalizable, or the ratio is the normalizing ratio itself), but *not* for isobaric interferences. Real-time ratios are for display purposes only, and are not otherwise used by *Analyst*.

❸ Rate of beam-growth or decay, updated after each peak-jump.

❹ Count-down of number of seconds remaining on the current peak for the current set.

❺ Background and interference-monitor peak graphics. The stippled region indicates the expected range of true zero (no-beam) readings; the measured backgrounds are indicated by small crosses (cyan and red for before- and after-peaktop backgrounds, respectively). The mass-locations of each background reading are artificially dispersed about the actual (and invariant) mass for clarity (the "cups" bracketing these mass-positions indicate the degree of artificial dispersion used).

❻ Interference-monitor peak readings, also artificially dispersed about the actual mass. Because of the greatly expanded scale of the background graphics, only very small interference-monitor peaks can be shown.

The Block Printout

The printout for each block is designed to be as compact as possible, yet still contain all the information necessary for an experienced operator to detect any unusual conditions or problems during the block. The block printout can often be discarded soon after the run is completed, as the more compact **Run Summary** contains most of the pertinent information about the block and the final ratios.

Background values are printed out just under the FOCUS and MAGNET information, and pertain to the counts per second (cps) and noise (in cps, at the 2σ level) at each background mass-position. There are 100 cps per millivolt for the Faraday Cup and about 10,000 cps per millivolt for the Daly detector. So a Faraday Cup background printed out as **503/9** indicates a nominal zero value of 5.03 millivolts with a background (dark) noise of .09 millivolts per second. The backgrounds should always be in the range of 3 to 7 millivolts (300 to 700 cps), and the background noise should consistently be roughly 10 cps (.1 millivolts/second) for the Faraday Cup and 1-4 cps (.0001-.0004 millivolts/second) for the Daly. Excess background-noise or unequal backgrounds on either side of a peak will be noted in the block printout by *Analyst*.

You may notice that for several consecutive blocks of data, only a printout indicating the *after* (peaktop-jumping) backgrounds is given. This is because for such a consecutive sequence, the *after* peaktop-jumping backgrounds for block **N** is also used as the *before* peaktop-jumping backgrounds of block **N+1**, so long as the blocks are closely spaced in time and the filament-currents were not changed between blocks.

If isobaric interferences were possible (this is determined by the *Element* definition), there will be one or more printed lines under the backgrounds, such as:

```
Average 85 Peak = .0736 mV;   Correction on 87 = .0561%
```

This line would indicate that an average of .0736 millivolts of an 85 peak was present during the block, and that the calculated amount of isobaric interference on mass 87 was .0561% of the *corrected* 87 peak.

If a linear regression of the ratios during the block indicates that there was a significant drift in the ratio with time, this drift will be indicated by a line such as:

```
<<< Ratio change during block of .012% Per minute >>>
```

A ratio drift probably indicates either rapidly-changing fractionation (for un-normalized ratios), the presence of a significant isobaric interference that is rapidly growing in or dying away, or growing/dying non-sample contamination of the element being run.

The **Time Constant Correction** in the printout is the applied correction, in ppm of the ratio, for the time constants ("memory" effect) of the amplifier. In general, this correction will be smaller than the accuracy of the ratio, but if you think that it's invalid, you can re-calibrate the time constants as described in the **Reference** section.

If the ratio were corrected for mass fractionation, the *uncorrected* ratio (**Discr.-Raw ratio**) is also printed out to the right of the time constant correction.

If the block were taken with the Daly detector (but not fractionation-normalized), the mass-discrimination factor applied for the Daly bias is printed out, as well as the nonlinearity constant for the Daly.

The significance of the rest of the block printout is as follows:

Heading	Significance
Mean 87/86 (or other ratio)	The final and corrected "mean" value of the ratio.
Set %error (obs.)	The "2σ" variation of the ratios of the individual sets of the block, in percent. In parentheses if better than or indistinguishable from the theoretical error.
Set %error (theor.)	The predicted 2σ variation of the sets, in percent, assuming a perfectly stable beam.
%error of mean	The 95%-confidence limit error, in percent, of the *mean* of the ratio, calculated from the **set %error (obs.)**, the noise of the backgrounds, the uncertainty introduced by the fractionation correction, and the uncertainty introduced by the isobaric-interference correction. This is a measure of the expected block-to-block reproducibility.
abs. error of mean	Same as **%error of mean**, but absolute rather than percent.
Delta%	The difference, in percent, between the ratio of the present block and that of the last block. In parentheses if this difference is not statistically significant.

Analyst uses *Tukey's Biweight* estimators to calculate the "means" and errors of the blocks, rather than means and standard errors. For blocks with set-ratios that conform to a normal distribution, this method yields results very similar to (and essentially as efficient as) means and standard errors. However, Tukey's Biweight estimators are far more resistant to outliers (or other types of non-normal distributions) than either a simple mean or an iteratively-trimmed mean (for example, by 2σ rejection), as well as distinctly more efficient than the more-simply calculated median. The algorithms are adapted from Hoaglin and others (1983, chapters 11 and 12). The "Outliers" number printed out for data blocks does *not* mean that any measurements were actually rejected, just that the number of sets indicated fell more than 2.5 "σ" from the "mean" (in quotation marks because these terms are not quite comparable for Biweight estimators). No data is actually rejected using the Biweight algorithm -- outliers are simply given a very low weight.

Using Isotope-Ratio Data Stored on Disk

After each block, the block's run-data is stored temporarily in the RESULT file (readable only from HT Basic) in the DATA directory. When the run number is incremented (because sample is changed or by user request), the run data (called a *Run Summary* by *Analyst*) is transferred to a RUN*nnn*.DAT file[1] in the RUNS directory. The numbers represented by *nnn* start at 000 and end at 999, after which the run-file counter resets to 000 again. Thus data for the last thousand runs always remain on the disk. The name of the run-data file that will be used is printed out before the first block's data for every run. A directory for the current *run* numbers (as opposed to *run files*) is kept on disk, so that you can request Weighted Averages by run number (run numbers range from 1 to 48, and are reset to 1 at the start of each new sequence of automatic runs). You can examine the sample names and dates of any or all of the RUN*nnn*.DAT files from the *Data Locator* routine (**F6** from the **Shift F8 Data** menu below, or **Ctrl L** from the *bms*). To get a display or hard copy of the run data for any run number or RUN*nnn*.DAT file, press **F3** from the **Data** menu (or just **R** from the *bms*).

```
                    Data Menu

F1  -- Start taking isotope-ratio data
F2  -- Enter names for all samples in a barrel            {E}
F3  -- Print/Display Run Summaries                        {r}
F4  -- Printout Run Overviews for auto-runs               {shift R}
F5  -- Calculate weighted averages of ratios for a run    {A}
F6  -- Locate run data on disk                            {Ctrl L}
F7  -- Show currently-defined sample-names                {N}
F8  -- Increment run# (without changing sample)
F9  -- Change sample name or spike# for this run
F10 -- Change Background-mass (until next ELEMENT change)
```

Run Overviews

If the information in the *Run Summary* is more than you need, you can request an even more concise record, *for completed automatic runs only*, called a *Run Overview*. A *Run Overview* includes just the Weighted Averages information for the run (all errors at the 95%-confidence level), and looks like this:

```
-----------------------------------------------------------------
Run# 12        Sample# 16                12 Jul, 1988
HYX-307 OPX, 30 min. warm HCl leach

                      abs.      %                          #blocks
 Ratio    Average    error     error  excess %err    mswd   rejected
143*144   .511905   1.2E-05   .0023%    .0015%       1.6    2 of 16
Sam/Spk    10.94     .014      .13       none        .86    1 "  "
-----------------------------------------------------------------
```

[1]The RUN*nnn*.DAT files are stored as tab-delimited DOS text files that can be imported into almost any DOS or MAC spreadsheet program.

To get a Run Overview for one or more automatic runs, either press **Shift R** from the *bms*, or press **F4** from the **Data** menu (**Shift F8** from the *bms*).

Weighted Averages of Isotope Ratios for a Run

Press **F5** from the **↑F8 Data** menu, or just press **A** directly from the *bms*. The screen will then show:

```
WEIGHTED AVERAGES OF RATIOS

F1 Screen Only
F3 Type in values to average by hand
Up/Down Arrow - Select file from list

Which Run#?  [press Enter for current run (#4)]

Display results only; press F1 to change...
```

If you want to average data for the current run (the one that you're still running or have just finished running), press **Enter**. To average data for some other run, enter that run number, or select from the list of RUN.*nnn*.DAT files (shows the last thousand runs by date and sample name) by pressing the up- or down-arrow. You can also type in data to average with **F3**. Note that you must enter errors for typed-in data at the 95%-confidence level (or 2σ if the number of measurements for each data-point is large).

When you've specified a run, *Analyst* will ask you to select one of the run's isotope ratios for averaging. When you've specified the isotope ratio, the screen will display a list of all those ratios for the run. You can reject any of the ratios for averaging at this point. You can then reject any of the data (by block) in response to the query:

```
Reject block #s?  (use - and ; as delimiters)
Example: 2-4;7;9;12-14 rejects sets 2 3 4 7 9 12 13 14          Alt-R=Recall
```

To reject any number of individual, specific blocks, separate those block-numbers with semicolons: for example, **2;4;6;8** to reject data for block numbers 2,4,6, and 8. To reject one or more continuous ascending series of blocks, separate the first and last block-numbers of the series with a dash: for example, **7-11** rejects block numbers 7,8,9,10, and 11. You can combine the two conventions, as in the example above.

Analyst will then calculate the weighted averages using an algorithm that:

1) First weights the ratios according to the inverse square of their errors;

2) Calculates the probability that the actual block-to-block scatter is due to the within-block errors alone;

3) If this probability is low, calculates how much block-to-block variance in excess of the within-block variance must exist, and recalculates the weighted average based on a weighting that combines the within-block and excess block-to-block variance;

4) Rejects ratios which are judged to be outliers and recalculates the average. Rejected ratios are indicated in the weighted-averages graphics by an empty or blue error-box (or a small circle if the error-boxes are very narrow). The rejection algorithm pays attention mainly to *excess* scatter of a data-point (that is, the deviation from the mean in excess of that predicted by its assigned error), but also permits easier rejection of a) first-block ratios, and b) ratios for blocks preceding or following blocks with rejected ratios.

If the calculated probability is less than 10-15%, there is probably some reason besides just the beam noise that caused the ratios to scatter from block to block. If the *Element* is not a fractionation-normalizable one, the excess scatter is probably due to changing mass fractionation.

The **M.S.W.D.** value in the weighted-averages printout refers to the Mean Square of Weighted Deviates. This does not refer to porcine perverts; it is the sum of the squares of the ratios of the residuals for each ratio divided by the estimated uncertainty of the ratio, all divided by N-1 (N is the number of ratios used). The M.S.W.D. value will be 1 on the average, if the within-block uncertainty accounts for all of the block-to-block variation. Values higher than about 2 for fractionation-normalized runs are a clear reflection of some sort of problem - either uncorrected isobaric interferences or hardware defects. A common example of uncorrected isobaric interferences arises when a sample has been total-spiked for both the running element and the interfering element (common for Sr and Nd samples), but the interfering element was not completely eliminated during the chemical processing.

The Weighted Averages graphics displays the averaged data in the form of error boxes for the ratios, graphed versus the time of the block for the ratio. These graphics can be very useful in evaluating the overall quality of a run.

Handy-Dandy Functions for Isotope Geologists

If you work with geochemical applications of Pb, Sr, or Nd isotopes, there are a few functions available from the *bms* that might occasionally be useful to you for "scratchpad" calculations, as follows.

Calculation of Radiogenic $^{207}Pb/^{206}Pb$ Ages: -- Press the equals key (=) from the *bms*. Enter either a radiogenic $^{207}Pb/^{206}Pb$ ratio (1 value) or the $^{206}Pb/^{204}Pb$ and $^{207}Pb/^{204}Pb$ ratios uncorrected for common-Pb (2 values, separated by a comma). In the latter case, the common-Pb ratios are assumed to lie on the Stacey-Kramers growth-curve for the calculated age.

Calculation of Model-Pb Age and μ: -- Press **Ctrl P** from the *bms*. Enter the $^{206}Pb/^{204}Pb$ and $^{207}Pb/^{204}Pb$ ratios of interest. The program will calculate a model age and μ ($^{238}U/^{204}Pb$ normalized for U-decay to the present day) assuming a Stacey-Kramers single-stage growth-curve.

Calculation of Model-Nd Age: -- Press **Ctrl N** from the *bms*. Select whether you want the model age calculated assuming a chondritic source with constant Sm/Nd, or assuming a depleted source. Enter the $^{147}Sm/^{144}Nd$ and $^{143}Nd/^{144}Nd$ ratios of the sample. You can adjust the parameters of both the chondritic-source model and the depleted-source model to correspond to both your geologic assumptions and laboratory normalization.

Calculation of Model-Sr Age: -- Press **Ctrl S** from the *bms*. Similar to the calculation of a model-Nd age, except that the depleted-source option is not offered.

AUTOMATIC RUNNING

If you can describe to another person roughly how to run one of your samples, in terms of what beam they might expect at what filament currents and how precise the data is to be, then you can do the same with *Analyst*, and have your routine runs (those without *gross* unpredictability) done automatically with no loss in quality compared to fully-attended run. This statement is based on extensive personal familiarity with fully-automatic runs for Pb, U, Th, Sr, Rb, Nd, and Sm. Many types of runs will actually give *better* data with fully-automatic running, because automatic runs tend to be done more reproducibly and in a more patient manner than manual runs.

Invoking Automatic Running

To start automatic running, press **F9 Start AutoRuns** from the *bms*. *Analyst* will then guide you through a few preliminary queries (Are your auto-run variables defined? Is the high-voltage correct for all runs? Does the printer have enough paper? Do you want any aborted runs to be re-tried at the end of the runs?), then begin the runs. But most important, you will have to define a set of **Run Variables** for the set of runs that you want done.

What Will You Have to Know to Do an Automatic Run?

Not very much. Much of the information has already been defined for the *Element* files (reference isotope, fractionation normalization, isobaric interferences...) and possibly the SPIKE files (normalizing isotopes and ratios, spike ratios...). Besides this, the most important things that you'll need to know are:

- At what filament current to expect at least a small beam,
- How fast you can take the filament(s) up to this current,
- How intense an ion beam you'd like to have,
- How intense an ion beam you'll accept if you can't get what you'd really like,
- How precise you'd like to have the data,
- If a triple-filament run, what criterion to use to determine the current of the center filament; the center-filament current only, the ^{187}Re beam, or the beam for the element of interest with no side-filament current.

Defining Run Variables

To tell *Analyst* how to do an automatic run, you'll need to define a set of **Run Variables** for each run. To invoke the **Run Variables** menu, press **Shift F9** from the *bms*. Or, press **F9 Start AutoRuns** from the *bms* and tell *Analyst* that your run variables are undefined when asked. The **Run Variables** menu will appear on the screen as shown below.

```
Automatic-Run Variables Menu

Help (what are Run and Std-Run variables?)
How to define Outgassing variables

Define a New set of Run Variables (deletes old)
Edit or view Run Variables
Add to Run Variables
Printout all Run Variables

Delete a Run
Insert a Run
Swap Run-orders

Add to Std-Run Variables
Edit or view Std-Run Variables
Printout all Std-Run Variables
Delete a Standard-Run

Press Green letter-key or Shift + Magenta letter-key;

press ENTER to retain changes & return to BMS, Esc to cancel
```

If you were going to define a set of **Run Variables** for a newly-loaded barrel, you would start with N. Try this now. The screen will then display the Run Variable *Form*, as in the example below.

```
RUN#  1                                  Barrel# ---> 12
Element ...   U/Th                       Isotopes     235,233,236,234
Sample Name:  Coral Standard #12, 1-column, not calcined

Single(1)-Triple(3)          3           Min. Beam (v)                .01
Focusing Isotope (CF)        187         Max. Beam (v)                .02
Center-Fil. Beam (v)         .25         Default Curr. (amps)         2.5
Initial CF (amps)            4.5         Default Beam (v)             .005
Daly Enable (0,1,2)          1           Fil. Incr/Block (amps)       0
Current-1 (amps)             1.4         Min# Blocks                  4
Rate-1 (mA/sec)              10          Max# Blocks                  8
Wait-1 (min.)                3           Error target (95%-conf%)     .15
Current-2 (amps)             2.25        #Sets/Block                  15
Rate-2 (mA/sec)              4           Max. Growth (%/minute)       7
Wait-2 (min.)                2           Preheat CF (amps)            3.1
Data-Wait (min.)             0           Preheat SF (amps)            1.8
Abort Current (amps)         3.1         NormSpike (0 if none)        12

ENTER each value, CTRL ENTER or F12 when complete, ESC when all runs defined

1 Help        2 Elements    3 Std Runs     4 Spikes       5 Integr/Delay-T
6             7             8 Sample-Outgas 9 Preh-Outgas 0
```

The values in the run-variables form above are obviously just examples: when you ask to define new run-variables, double question-marks that indicate "you must enter a value" will appear instead. But note that:

1) The double question-marks will only appear for the first run of the several you would typically define (one for each sample). After you define the parameters for the first run of a series, the next run you define will inherit the values you typed in for the previous run as their default values. So if all of your runs were to be run in a similar way, you would need to enter only the barrel number for all but the first run[1];

2) There will usually be **Standard-Run Variables** defined that closely approximate the kind of run that you want to do, and you can get a list of **Standard-Run Variables**, then select one to copy into the Run Variable form by simply pressing **F3** (see the section on Standard-Run Variables, below);

3) Though the names for the various run variables are admittedly cryptic, a HELP screen (press **F1**) will explain the use the particular run-variable that the parameter-cursor is on.

Overview of an Automatic Run for Single-Filament Samples

Before going further in this explanation of the Run Variables, we should briefly go over how the automatic runs will be done by *Analyst*. First, of course, the sample at the specified **Barrel#** will be rotated into position. If for some reason good filament-contacts are not obtained at this point, *Analyst* will try a second time to rotate the sample into position and re-test the contacts; if a second contact failure occurs, the run will be aborted.

Preheat Filaments: -- If you specified nonzero values for the **Preheat Cf** and/or **Preheat Sf** variables, the preheat filaments will be taken to the specified currents at a rate that starts at 30 milliamperes (mA) per second and decreases in steps to 1 mA/second as the target current is approached. The preheat filaments will be held at these currents for two hours or until the run is over, whichever comes first.

First Filament-Current Take-Up: -- The filament current will be raised to **Current-1** amperes at a rate of **Rate-1** mA/second[2] and left there with no action for **Wait-1** minutes. After **Wait-1** minutes, the filament current will be taken to **Current-2** amps at a rate of **Rate-2** mA/second.

Obtaining a Usable Beam: -- Unless a "Tuneup Isotope" is specified (p. 37), *Analyst* will then quickly scan over all of the nuclides in the **Isotopes** list of the Run Variables, and determine the Most-Intense Peak (**MIP**). If a usable beam (of either the MIP or the Tuneup Isotope, if defined) is present (that is, more than a few tenths of a millivolt and reasonably stable), *Analyst* will center the **MIP**, focus the ion optics, and optimize the barrel position. Otherwise, *Analyst* will increase the sample-filament current (if the beam is too small) or wait (if the beam is dying or unstable) until a usable beam is obtained.

---

[1]If, as I strongly recommend, you entered all of the sample names just after changing the barrel, the sample names will automatically appear as the default sample names for the runs as soon as you specify the barrel number for the run.

[2]But if the filament had previously been outgassed in the preheat position, the rate will be <u>double</u> the specified rate until the sample-filament current reaches the preheat current.

By increasing or decreasing the sample-filament current, *Analyst* will attempt to adjust the **MIP** beam until it lies within the window defined by the **Min. Beam** and **Max. Beam** values. If the sample-filament current exceeds the **Default Curr.** parameter in this attempt, however, the minimum acceptable **MIP** beamsize becomes the **Default Beam** value. The **Default Curr./Default Beam** Run Variables can be very useful, so you should understand what their purpose is and how to use them. In essence, these variables should be used to accept an alternate beamsize if the size of the beam at a given current indicates that the beamsize you'd really rather have will not, in fact, be obtainable.

For example, suppose that you expect at least a 3-volt beam of 206 for your zircon-Pb run. But the zircon turns out to be much younger than you had expected, or perhaps the chemistry was bad for some reason, so the filament-load just cannot give any more than an 800 millivolt beam. If data from an 800 millivolt beam would be better than aborting the run and getting no data at all, you would want the **Default Beam** Run Variable set at something less than 800 millivolts, and the **Default Current** set at some value towards the normal upper limit for your Pb runs. This **Default Current** value must fall between the **Abort Current** and **Current-2.**

Using an arbitrary peak ("Tuneup Isotope") for beam tuneup and beam-size adjustment: You can specify that any nuclide defined for the *Element* of a run be used instead of the **MIP** for beam-tuneup and to satisfy the **Min. Beam, Max. Beam,** and **Default beam** parameters. This nuclide is called the *Tuneup Isotope*. To do this, type in the **Min. Beam** value followed by a slash and then the isotope that you want to use. For example, consider a run with ratio-data for the 233, 234, 235, and 236 peaks. As these are all low-abundance isotopes, you might want to use the major isotope (^{238}U) for beam-tuneup rather than the most abundant of the data-taking isotopes. Assuming that you wanted at least 1.2 volts of 238 for data-taking, you would then enter **1.2/238** for the **Min. Beam** parameter.

The DATA WAIT: -- Once *Analyst* has obtained a beam that satisfies the beam-window criteria of the Run Variables, you can specify a final wait-period before taking data. This final wait is the **Data Wait** parameter of the Run Variables. You can use this wait, for example, to provide an additional time for mass fractionation to settle down to a reproducible value. The main difference between **Data Wait** and **Wait 2** is that the **Data Wait** occurs *after* any filament-current changes required to satisfy the beam-window parameters. Another important difference is that excess beam-growth is monitored during this WAIT (if excess beam-growth occurs, the sample-filament current will be reduced), so you can use this time to allow the beam to grow in without risking catastrophically rapid growth. Growth-rate monitoring is disabled, though, if the beam falls below the **Default Beam** size.

Final Scan: -- Just before starting the first block of data, *Analyst* will quickly scan over the isotopes again to determine the optimum peak-switching sequence, integration times, and delay times. The number of sets in each of the data blocks are specified by the **#Sets/block** variable.

Checking for Beam Size and Growth Rate: -- After each block, *Analyst* will check the **MIP** (or Tuneup Isotope) beamsize and the rate of beam-growth or decay during the block. If either the beamsize or growth-rate lies outside the values specified in the Run Variables, *Analyst* will raise or lower the sample-filament current in response. In cases of extreme beam-growth, defined as more than twice the specified limit, *Analyst* may intervene in the *middle* of block to turn down the filament-current. Such within-block intervention is forbidden from occurring more than 4 times in a run, however.

Between-Block Filament-Current Change: -- If the sample-filament current were *not* changed to control the beamsize or growth-rate and if the **Fil Incr./Block** Run-Variable were nonzero, the sample-filament current will change (generally, increased) by the **Fil. Incr./Block** value.

Keeping the Beam Focused: -- *Analyst* will focus the beam (MIP or Tuneup Isotope) after the first block, then every fourth block. The barrel position will be optimized every sixth block for single-filament runs, but only before the first block for triple-filament runs. If, however, a triple-filament run experiences filament-contact problems at any point, no further barrel adjustments will be attempted. You can also limit the number of barrel-centers that will be attempted during each automatic run from the **↑F3 Barrel** menu from the *bms* **(F10 Inhibit Center)**.

How Many Blocks of Data?: -- The number of blocks of data that will be taken depends on the **Min# Blocks** and **Max# Blocks** variables, together with either the **Max %error/block** or **Error Target** variables. Unless the run is aborted, *Analyst* will take *at least* the **Min# Blocks,** but no more than the **Max# Blocks.** Once the run has accumulated the **Min# Blocks,** the number of additional blocks will be controlled by one of two possible approaches:

Terminating Criteria for *Elements* without Fractionation-Normalization: (*excluding* non-normalizable *Elements* that were defined as "Can Be Double-Spiked") -- After each block, *Analyst* will determine how many of the blocks meet the criteria imposed by the **Max %error/block** variable. If this variable is *negative*, then for a block to count towards the **Min# Blocks** criterion, the uncertainty of each of the ratios of the block must be less than the absolute **Max %error/block** value. If this variable is *positive*, ratios with precisions that are within theoretical limits for that ratio will also be acceptable.

Normally, you should enter a *positive* value for the **Max %error/block** variable. You can then demand a high precision for ratios of the most-abundant isotopes, while still accepting ratios for one or more minor isotopes. For example, consider Pb-isotope ratios for isotopes 206, 207, and 204 where the 206/207 ratio is about 10 and the 206/204 ratio about 1000. In most cases, the precision of the 206/204 ratio for any block will be entirely controlled by the theoretical limits[1] on measuring a small peak, and therefore by the beam-limits that you specify for the run. Only the 206/207 ratio will be sensitive to instability, so in this case a *positive* **Max %error/block** variable will in effect pay attention only to the 206/207 ratio, and so can be much more sensitive to blocks with unstable beams.

Terminating Criteria for Runs with Fractionation-Normalization: (*including* non-normalizable *Elements* that were defined as "Can Be Double-Spiked") -- For runs of *Elements* such as Sr and Nd, *Analyst* will terminate the run depending on the ultimate precision for a "critical ratio" of the run. This ultimate precision refers to the precision that is obtained from a weighted average of the "critical ratio" for *all* of the blocks of the run. The Run Variable that specifies this precision is the **Error Target (95%/conf%)** variable, for which you enter the desired overall precision of the "critical ratio" in percent and at the 95%-confidence level. The "critical ratio" is defined by *Analyst* as either the radiogenic-isotope ratio (for example, 87/86 or 143/144) if one exists, or the SAM/SPK ratio if not.

For each block after the **Min# Blocks,** *Analyst* will do a weighted averages of the "critical ratio" to see if the overall precision of that ratio meets or exceeds the **Error Target (95%-conf%)** criterion. As soon as this is the case (or when the **Max# Blocks** has been reached), the run will terminate. So by using this approach, you can specify the overall precision that will be obtained by each run, without having the run spend any unnecessary time taking data once a satisfactory level of precision has been obtained. For example, if you want a 95%-confidence level precision on the 87/86 ratio of about 0.00002 for each strontium run, you would specify an **Error Target (95%-conf%)** of .003% (assuming an 87/86 ratio of about 0.7).

If you want to be rather tricky, *Analyst* has a feature that will allow you to define an automatic run that will take both "insurance" data and, if possible, high-quality data. To do this, just enter the **Default beam** as its *negative* value. A negative **Default beam** (the negative sign is used only to indicate the procedure described here; all values

[1]Remember that you can tell if the precision of a ratio is within the theoretical limits for that ratio by looking at the SIGMA% OBS. value in the block printout. If the precision is within theoretical limits, it will be printed out in parentheses.

are taken as positive) indicates that once the **Min# blocks** has been obtained, *Analyst* is to check to see if any of the blocks were obtained with less than the **Min. Beam** beamsize (that is, with only the **Default beam**). If so, *Analyst* will increase the sample-filament current(s) to try and obtain the **Min. Beam** beamsize (regardless of the **Default current** value), and then attempt to take enough additional blocks to satisfy the original **Min# blocks** specification.

For example, consider a run specified with **Min# blocks** = 8, **Min. Beam** = 2000 mV, **Default curr.** = 2.4 amps, and **Default beam** = - 150 mV. After 8 blocks of data at 200 mV and 2.45 amps, *Analyst* would increase the filament-current to obtain a 2000 mV beam. If successful (an abort would be possible, of course), *Analyst* would then take *another* 8 blocks -- but this time at 2000 mV. If the run aborted in the attempt, nothing but a little time is lost and you would still have some useful data. If successful, you would have significantly better data than if you had just played it safe.

*You can also use negative **Default beams** to force **Default beam** data to be taken on the Daly detector, even if the assigned **Max. Beam** value were several volts. To do this, enable the Daly detector for data-taking in the Auto-Run Variables form, and specify the negative **Default beam** to be no more than 35 millivolts. If the **Max. Beam** is more than 50 millivolts, then when the **Default beam** data are taken, the **Max. Beam** will be temporarily re-assigned a value of 44 millivolts, which will ensure that all of the **Default beam** blocks will be taken on the Daly. When* Analyst *later attempts to get **Min. Beam** data-blocks, the **Max. Beam** parameter will revert to its initial value.*

End-of-Run Procedures: -- At the end of each run, *Analyst* will print out a run summary for the run (as described in the Manual Running section) and weighted averages (including a graphical display of the ratios and precisions for each block of the run) for each of the non-normalizing ratios of the run. The Weighted Averages information is stored disk for later retrieval as a Run Overview. When automatic running is completed (at the end of the last-defined automatic run), *Analyst* will print out a Run Summary for each of the runs, and then a Run Overview for each of the runs.

Overview of an Automatic Run for Triple-Filament Samples

For samples loaded on a triple-filament assembly, *Analyst* will take up the center-filament current before taking up the side-filaments. There are three strategies that you can specify for controlling the center-filament current during the run. These strategies depend on the values for the **Focusing Isotope, Center-fil Beam,** and **Initial-cf** Run Variables (these Run Variables will appear only if the run is designated as a triple-filament run).

The first strategy, and the simplest, occurs when the **Focusing Isotope** and **Center-fil Beam** variables are set to zero. In this case, *Analyst* will take the center-filament current to the **Initial CF** amps, and leave the center filament at that current for the rest of the run. This strategy is appropriate for runs where the center filament not hot enough to yield a measurable rhenium beam, and also not hot enough to yield a measurable sample-element beam with side-filament currents of zero. The disadvantage of this strategy is that the center filament temperature for a given current can vary significantly from run-to-run due to variations in filament thickness.

The second strategy is to specify the size of the ^{187}Re beam during the run. This strategy is useful in cases where the center filament is a rhenium filament and where the temperature of the center filament will be hot enough (more than about 1850°) to yield a measurable ^{187}Re beam. To specify this strategy, set the **Focusing Isotope (CF)** to 187, the **Center-fil Beam** to the desired ^{187}Re beam, in volts, and the **Initial CF** to the approximate current that should yield the desired ^{187}Re beam. *Analyst* will start looking for a ^{187}Re beam at the **Initial CF** current, focus on the peak, then raise or lower the center-filament current until the **Center-fil Beam** is obtained. *Analyst* will check

the ^{187}Re peak before each subsequent block, and adjust the center-filament current to maintain a constant ^{187}Re beam. This strategy is useful for triple-filament runs of very refractory elements, such as U, Th, and Hf.

The third strategy is to specify the size of the peak for an isotope of the element being analyzed, with the side filaments turned off. In this case, specify the **Center-fil Beam** as for the second strategy, and specify the **Focusing Isotope (CF)** as the major isotope of the *Element* of interest. After taking the center filament to the **Initial CF** current, *Analyst* will slowly raise or lower the center-filament current until the beamsize of the **Focusing Isotope (CF)** matches the **Center-fil Beam** value. Once this condition is met, *Analyst* will take up the side-filament currents and make no further changes in the center-filament current. This strategy is very useful for relatively non-refractory elements such as Rb, K, Sr, and Ca.

More Information about Specific Run-Variable Parameters

The *Element* Parameter: -- The name of the *Element* that will be assigned to the run. Select *Element* from the list of defined *Elements* by pressing **F2**. Remember that the *Element* file contains all the necessary information on the proper accelerating voltage, magnet settings, fractionation normalization, isobaric interferences, and background location.

The *Isotopes* Parameter: -- These are the isotopes or nuclides that you want to take isotope-ratio data for, separated by commas. *Don't* include isotopes that will be used only for correction of isobaric interferences: these should already be defined in the *Element* file. You can enter up to 8 isotopes. If the *Element* is one with internal fractionation-normalization (such as Sr, Nd...), the isotopes list must contain both the **Reference Isotope** (such as 86 for Sr) and the **Normalizing Isotope** (such as 88 for Sr). And, if the sample were spiked with a spike that is defined on disk, the ISOTOPES list must also include the third nonradiogenic isotope specified in the definition for that spike (such as 84 for Sr).

The *Sample Name* Parameter: -- The name (up to 50 characters long) that will be assigned to the run. If the names for the samples in each barrel position were defined before entering the Run Variable *Form*, the appropriate name will appear automatically as soon as you enter the barrel-number for the run. Of course, you can change this default name to something else if you like.

The *Daly Enable (0,1,2)* Parameter: -- Specifies if and how the Daly detector is to be used in the run. A value of ***0*** indicates that the Daly is not to be used under any circumstances (remember: don't enter 0 unless the Daly is really nonfunctional). A value of ***1*** indicates that the Daly can be used for beam tuneup, and also for data-taking if the peaks for all of the data-taking isotopes are less that about 45 millivolts. A value of ***2*** indicates that the Daly can be used for beam tuneup, but *not* for data-taking under any circumstances.

The *Preheat CF* and *Preheat SF* Parameters: -- These variables specify the currents to which the filaments of the filament-assembly in the *preheat* position will be taken. If the variables are nonzero, this will happen just after the *sample* filament-assembly is rotated into running position. The preheat filament-currents (CF=center-filament, SF=side-filament) will be maintained for the length of the run or two hours, whichever occurs first.

The *Normspike* Parameter: -- If the run were for a fractionation-normalizable *Element* and the sample were spiked with one of the spikes defined on the disk in the DATA directory (p. 55), this variable specifies the number of that spike (a value of 0 indicates an unspiked sample). The data for each block will then be corrected for fractionation and spike isotopes, and the sample/spike ratio will be calculated (p. 25). Select from the list of defined spikes by pressing **F4**.

Auto-Run Operator-Specified Integration/Delay Times: -- As for manual data-taking, you can over-ride *Analyst*'s choice of integration and delay times for the data-taking peaks (see discussion on page 21). Press **F5 Integr/Delay-T** at any point during entry of the run variables to toggle between *Analyst*-calculated and operator-specified times. For operator-specified times, you will be asked to enter the integration/delay times just after you enter the run-variable *Form* with **F12** or **Ctrl Enter**.

Using Standard-Run Variables

Standard-Run Variables are Run Variables that are typical for several different types of runs and that can be placed in a Run Variables *Form* with a few keystrokes. For example, suppose that you're defining Run Variables for a barrel of both unspiked and spiked common-Pb samples, and that the sample you want to run first is one of the unspiked samples. Suppose also that someone (perhaps you) has already defined a set of the Standard-Run Variables to match the way you want to run your unspiked samples. You could then copy the Run-Variable parameters from that Standard Run into your Run Variables by pressing **F3 Std Runs** from the Auto-Run Variable *Form*, and make the few changes required to match the particular run you had in mind.

So the Standard-Run Variables are used to define and store *typical* ways of running different kinds of samples, so that they can be invoked whenever one of your runs will be reasonably similar to one of the Standard Runs. By using the Standard-Run Variables instead of filling the Run Variable *Form* from scratch, you can save time and avoid simple typographical errors.

You can define up to 32 Standard Runs. To examine Standard Runs, either print the complete set out by pressing **Shift P**(rint) from the Automatic-Run Variables menu, or press **Shift E**(dit) to examine them one by one.

Defining Standard-Run Variables

Standard-Run Variables are defined in the same way as Run Variables. Just use the shifted keys defined in the Automatic-Run Variables menu that refer to Standard-Run Variables, instead of the unshifted keys that invoke routines for Run Variables. The only difference compared to defining or editing Run Variables is that the *Form* for each Standard Run will ask for a **STD-RUN#** instead of a **RUN#** and a **STD RUN NAME** instead of a **SAMPLE NAME**, and that no barrel-number will be requested.

Intervening During an Automatic Run

You can intervene during an automatic run to perform some series of actions, then return to the automatic run where it left off. For example, once you have temporarily exited to the *bms*, you can scan the isotopic spectrum, change filament currents, focus the ion beam, calculate weighted averages, or even change the Run Variable values for the run in progress. About the only things that you *can't* do while temporarily exited from automatic running are to:

- ➤ Change the barrel-number specified in the Run Variables,
- ➤ Change samples during the run,
- ➤ Change the *Element* of the run, and
- ➤ Take data in the manual mode.

To temporarily exit from automatic running once automatic running has begun, wait until **F1** is labelled **→Manual** at the bottom of the screen. When you press **F1 →Manual**, *Analyst* will (within a second or two) exit to the familiar *bms*. You can then invoke any of the functions of *Analyst* (with the above exceptions) just as if you were in the manual-running mode. When you're ready to revert to automatic running, press either **Home** or **←Backspace** from the *bms*, and *Analyst* will continue the automatic run from where it left off (or from the beginning of a data-block if interrupted in the middle of one).

If you want to exit an automatic run and re-enter automatic running by beginning at some *other* run instead of the one that was in progress, press **Shift HOME** instead of **HOME** from the *bms*. You can then specify that *Analyst* re-enter automatic running at the beginning of *any* of the runs defined in the current Run-Variable list. With this option, you can completely re-run one or more samples, or skip several runs.

If you don't want to just *temporarily* exit from the automatic run, you have two other options: quitting just the current run, or leaving the automatic-running mode entirely. To quit the run in progress, press **F2 →Next Run** (when so labelled at the bottom of the screen) during the run. When you confirm this request, *Analyst* will immediately end the run, print out the data, do weighted averages of any completed blocks, and then go on to the next automatic run.

If you want to terminate automatic running entirely, first exit to the *bms* by pressing **F1 →Manual**, then **F9 Auto←→Manual** from the *bms*. Select the Manual Running option that follows. You will then be back at the *bms* in the manual mode, and can finish the run as if it had started in the manual mode.

Remember to use **F1 →Manual**, *not* **Esc** to exit automatic running. Pressing **Esc** during automatic running simply terminates the immediate operation, such as focussing, peak-centering, or filament-current increase. This may be what you want to do in some cases (for example, if the beam were being focused but you were satisfied that the focus was already adequate), but unless you know what you're doing, could bypass an important operation.

Entering Automatic Running from the Middle of a Manual Run

You can start automatic running from the middle of the automatic-running sequence (that is, from the *n*th auto-run rather from the first-defined auto-run), or even revert to automatic running at any stage of a manual run.

For example, suppose you brought the filaments of sample 3 up to running temperature in the manual mode, tuned the beam up, and took a couple of blocks of data. Then you wanted to enter the automatic-running sequence starting at the third run, without losing any of the work that you had put into the sample already. To do this, you would press **F9** from the *bms* (Start Auto Runs). From the next screen display, select the **Start From?** option, and specify run **3** to start from.

Analyst, recognizing that the correct sample is already in position, that the filament-currents are already satisfactory, and that a few blocks of data have already been taken, will simply proceed with the automatic run as if it had started in the automatic mode in the first place. The transition to automatic running will be just as smooth even if the filament-currents are only partly towards their **CURRENT-2** target, or not turned on at all.

What Will Cause an Automatic Run to Fail?

Except for gross hardware malfunctions and software bugs, many of the causes for aborted runs are preventable, as listed below.

1) Wrong high-voltage setting for the *Element* being run (or drifting HV due to hardware malfunction). This will cause an abort without any attempt to run the sample (so the sample can be rerun). The tolerance is ±15 volts from the *Element*'s specified value.

2) Bad filament-contacts. If bad contacts are encountered, *Analyst* will try hard to improve the situation, either by slightly wiggling the barrel to rub off any bits of fluff or scale in the contact area, by completely resetting the barrel and re-finding the sample, or both. If none of these strategies succeeds in regaining filament-contact, though, *Analyst* will have to abort the run.

3) The Daly Detector was not completely turned on. If your runs assume the presence of an operating Daly Detector and you forgot to turn on the Multiplier Supply, the Brandenburg (and **RESET** the Brandenburg), and the FA3 amplifier (if present), the run will abort at an early stage.

4) Grossly unstable beam. If, at the time of the first beam tune-up, the beam is persistently very noisy (spiking) or growing/decaying extremely rapidly, the run will abort. Before aborting, though, *Analyst* will wait up to 15 minutes for the beam to stabilize. If the problem is a noisy (spiking) beam rather than a rapidly growing/decaying beam, *Analyst* will "flash" the filament after the 15-minute wait by rapidly increasing the filament current by 15%, waiting a few minutes, then returning the current to its original value. In many cases, this can restore stability to an otherwise hopeless run.

5) Wrong sample. Obviously, if you mistakenly specified the barrel number for a samarium sample instead of a neodymium sample, the run will be forced to abort due to insufficient beam.

6) Bad pressure. *Analyst* will wait up to an hour for satisfactory pressure (as defined from the **Hardware Configuration** form -- **Shift F6 F8** from the *bms*) to be gained in the source can and the flight tube, then give up and abort the run. This may happen if the cold-trap warms up mid-way through the automatic-running sequence.

7) Panel switches set to the wrong positions. Make sure the panel switches are set to the positions indicated in the **Reference** section, that the filament-current supplies and Brandenburg have been **RESET**, that the beam-valve (LOS valve) is open, and that the High Voltage is on.

Hardware malfunctions, of course, are out of your control. Because of the possibility of a hardware malfunction that could result in ruining every sample in a barrel, *Analyst* won't permit automatic runs for more than two samples in a row to fail without ever having attained a significant beam. In such a case, *Analyst* will suspend automatic operation entirely.

Automatic Outgassing Runs:

Analyst has a special kind of automatic run for outgassing filaments -- that is, to just take the filament(s) up to some target current at an arbitrary rate, then to wait at that current for an arbitrary time without any intention of taking data. These runs may even be done with the high voltage turned off and the beam-valve closed, to keep any crud that volatilizes from the filament away from the source assembly as much as possible.

Analyst recognizes an outgassing automatic run from the *Element* name OUTGAS or P-OUTGAS in the Run Variable *Form*. As soon as you enter either of these names as the *Element*, all of the parameters in the Run Variable *Form* that aren't relevant for outgassing (such as ISOTOPES, SETS/BLOCK, MAX.# BLOCKS...) are replaced by asterisks. Press **F8 Sample Outgas** from the Run Variable Form to specify that the filament-assembly in the *running* position (that is, directly in front of the source assembly) be outgassed. Press **F9 Preh Outgas** to specify outgassing of the filament-assembly in the *preheat* position.

An automatic outgassing-run will rotate the sample into position (running position if *OUTGAS*, preheat position if *P-OUTGAS*), take up the sample-filament current according to the **Rate-1, Current-1, Wait-1, Rate-2, Current-2,** and **Wait-2** parameters, and then go on to the next run.

Multiple Runs on the Same Sample

You can do more than one run on a given filament-assembly without turning off the filaments between runs and completely restarting a new run. *Analyst* refers to such runs as *Linked Runs*. For example, suppose that you wanted to take data for uranium, then raise the filament currents enough to grow in a thorium beam, and then take thorium data. Just define your usual automatic run for uranium, and then define the next run to be a thorium run for the same sample.

After completing the uranium run (but without turning the filaments down or off), *Analyst* will take the sample-filament (center if a single, sides if a triple) directly to the CURRENT-2 target if CURRENT-2 is greater than the sample-filament current at the end of the uranium run. If the sample-filament current at the end of the uranium run were already greater than the new CURRENT-2 value, *Analyst* will make no immediate change in the sample-filament current. The CURRENT-1/RATE-1//WAIT-1 variables of the thorium run will be ignored. *Analyst* will then adjust the thorium beam-size to the window specified in the Run Variables for that run, and begin taking data.

You can specify as many linked runs as you like for any given sample. The only restriction is that the total number of automatic runs for a particular suite of automatic runs be no more than 48.

You can use the linked run feature in cases where you don't want to really combine runs of different elements on the same sample, but just want to take different isotopes. For example, you might want to specify the first run for a sample as a Pb 206-207-208 run, and the next run on the same sample as a Pb 206-204 run at a higher beamsize and with different requirements on the precision and number of blocks.

Another use of linked runs is to ask for both moderate-quality and high-quality data, so that you get the best data that the sample is capable of giving. For example, for a sample of unknown loading-amount (and therefore unknown maximum-sustainable beamsize) you could ask for a run that will accept a minimum of 100 mV of beam, followed by a run on the same sample that will require a minimum of a 1000 mV beam. Once the first run is

successfully completed, this procedure will automatically go on to try and get higher-quality data. If it aborts during the second run, nothing will have been lost except a little time[1].

One danger of specifying linked runs is that if the first of a series of linked runs aborts because of insufficient beam, any chance of re-running that sample for the isotopes specified could be ruined by higher filament-currents attained during subsequent linked runs for different isotopes on the sample. However, *Analyst* will ask you if you are willing to assume that risk before your auto-runs are started.

Automatic Hardware-Diagnostic Checks

Before *Analyst* will begin automatic running, you will be asked to confirm that the accelerating voltage is valid for all of your runs, that the beam valve is open, and that the printer has adequate paper. This screen will also ask you to press **F5** if you want one or more diagnostic routines to be performed after or during the automatic runs. The diagnostics options that will be performed *after* the automatic runs are finished are:

1) Scan the entire mass-spectrum for the current *Element* using the Daly detector for small peaks and the Faraday Cup for large peaks (takes 1-3 minutes);

2) Scan from the most-intense-peak minus 0.5 mass-units to the most-intense peak (using the Daly detector) while the beam is small, then switching to the Faraday Cup) to determine both the abundance sensitivity and the resolution of the mass spectrometer (takes about a minute: see p. 57);

3) Do a quantitative (slow) peak-flat determination (takes about 20 minutes) using the most-intense peak (p. 58);

4) Calibrate the time constants of the amplifier system (takes 30-40 minutes; see p. 57);

5) Scan the focus-potentials for all plates, with graphics showing the ion-beam response, and also with graphics showing the DAC (digital-to-analog-converter) output response (takes about 10 minutes; bad DAC's will be diagnosed and noted),

6) Scan the magnet with graphics showing the Hall-Probe Output response (takes 1-2 minutes; apparent problems will be diagnosed and noted),

7) Check the stability and noise of the accelerating voltage (takes about 60 minutes; an unstable HV will be diagnosed and noted).

The diagnostic routines that can be performed *during* the automatic runs are:

8) Do a quantitative (slow) peak-flat determination using the most-intense peak (takes about 20 minutes) *after each* run (p. 58);

---

[1]Another way of achieving the same end for some types of runs is to specify a **FIL. INCR/BLOCK** value that will significantly increase the beamsize between blocks. If you also specify a large number of blocks, then you will almost certainly get the maximum-possible beamsize out of the sample. If this sort of procedure induces runaway beam-growth in the run and you have specified a **MAX. GROWTH** value, *Analyst* will reduce the filament-current as necessary and cancel any further inter-block filament-current increases.

9) Do a semi-quantitative (fast) peak-flat check, using the most-intense peak on the data-taking collector (takes about 15 seconds) *before* each block for *every* run (p. 58);

10) Scan the magnet over a specified mass-range before specified blocks for specified runs (takes 1-3 minutes per scan);

11) Check for stability of the magnet-positions (for the most-intense peak) during each block. This is *always* done, though unless the routine is specifically enabled the results are only printed out if there are obvious problems;

12) Check for stability of the accelerating voltage before each block for the run;

13) Show the drift/scatter of the backgrounds (for the least-intense peak) for each block of the run; and

14) Show the drift/scatter of the source-can and flight-tube pressures for each block of the run.

Routines 1 through 7 will be done using the last sample that was run in the automatic-running sequence. For routines 2, 3, 4, and 8, a peak of at least 5 volts will be required, and the computer will increase the sample-filament currents if necessary to get such a beam. So for these routines, make sure that the last sample is capable of yielding such an intense beam, and that you won't mind if the sample is ruined in the attempt.

All of the graphics for these routines, plus all pertinent numerical data, will be dumped to the printer. Additional information is given in the **Hardware Diagnostic Routines** part of the **Reference** section.

REFERENCE

Introduction

This part of the documentation contains specific information about some of the features of *Analyst* that aren't covered in the earlier sections. Though not the easiest way to find out how to use *Analyst*, this section will tell you about many functions that haven't been discussed so far.

Nonetheless, you won't find descriptions of all of the features and functions of *Analyst* in this section. In fact, you won't find information about some of the features anywhere in this User's Manual. Most of the features of *Analyst* are more-or-less self-documenting, however, and can be both located and used just by intelligently combining the information in the shifted-Function key menus, the *Forms*, and the HELP screens. I realize that this method of learning isn't very convenient if you need to perform some obscure function in a hurry, so I strongly advise you to take some time to sit down with *Analyst* and an expendable sample or two (or, more efficient, run *Analyst* in Emulation Mode -- see p. 2), stroll through all of the various menus and functions, and experiment with them.

Procedures for Starting a New Barrel

When you install a new barrel-load of samples, there are two things that you should do as a routine procedure: perform a contact-test for all of the samples (filament-assemblies) in the barrel, and enter sample-names for all of the samples in the barrel.

The CONTACT TEST Procedure: -- The contact-test procedure rotates the barrel past all of the samples, and gives you a graphic display of the contact-width of both the side and center filaments for each sample, both in the running position and the preheat position. You should do this as soon as you are ready to start pumping the source-can down. The procedure is to:

1) Install the face plate of the source can and the barrel-motor belt, then start the rough-pump;

2) Turn on the turbomolecular pump, wait until the Pirani gauge reads .01 microns or less, then turn on the high-vacuum gauge for the source;

3) Turn all of the filament knobs on the mass-spectrometer to RESET, then ON (both center-filament and side-filaments, both sample and preheats);

4) Turn the barrel-motor ON;

5) From the *bms* state of *Analyst*, invoke the ***Barrel*** menu with **Shift F3**, then press **F2 Check All** (or just press **B** during the *bms*);

Analyst will then reset the barrel, start rotating the barrel slowly so that all of the sixteen possible samples pass through both the sample and preheat filament-contact assemblies, and display graphically the regions where filament-contacts were made for each sample. The horizontal line at the zero position of the Y-axis indicates the default barrel-position for each sample. Solid magenta boxes to the left or right of the vertical line showing which sample is being tested indicate that valid contacts were found for both the center filament and the side filaments of that sample. Stippled white patterns indicate valid contact for a center filament only, and empty cyan boxes indicate valid contacts

for the side filaments only. Boxes to the left of the vertical line indicating the barrel-number indicate contacts in the running position; boxes to the right of the line indicate contacts in the preheat position.

If the region of valid contact is less than about 20 barrel-units, or if there are gaps in the contact region, it may be difficult for *Analyst* to either "find" the sample or to properly optimize the barrel once a beam is found. If less than 10-12 units of contact exist, you should either vent the source-can and determine the cause of the problem, or accept that you may not be able to get a run from that sample.

When the contact-test is complete, *Analyst* will ask you if you want to erase the previously-defined sample-names at this time. Normally, your answer should be YES, since otherwise *Analyst* will assign the sample-names for the previous barrel to this barrel's samples.

Entering Sample Names for a New Barrel: -- If you erased the previously-defined sample names after the completion of the contact test, as recommended above, *Analyst* won't suggest default sample-names for manual or automatic running, and won't display the sample names during the *bms*. Because not having the sample names displayed (and changed each time a new sample is rotated into running position) increases the risk of the operator trying to run the sample at barrel-number *N* when actually the sample at barrel-number *M* is in running position, I strongly recommend that you enter the names for each of the samples as soon as possible after you install a new barrel. To enter the sample names, bring up the ***Data*** menu with **Shift F8** from the *bms*, then select **F2 Enter Names** (or press **E** from the *bms*).

Defining a New *Element*

You'll need to define a new *Element* for *Analyst* if you:

1) Start running an element or ionic species that no one else has run before,

2) Decide to use a different pair of isotopes for fractionation-normalization or to use a different value for the normalization ratio,

3) Decide to use different isotopes to monitor for isobaric interferences or to use different values for the isobaric-interference ratios,

4) Decide to use a different reference isotope, or

5) Decide to use a different high-voltage setting for your runs.

If you need to define a new *Element* for any but the first reasons, you won't need a beam to do so. If you need to define a new *Element* for a new element or ionic species, however, you will need a beam unless the isotopes of interest overlap with some previously defined *Element*.

The NEW ELEMENT Procedure: -- Bring up the ***Magnet*** menu from the *bms* by pressing **Shift F1**, then press **F6 Define Element**. The screen will clear and display:

```
Magnet Calibration for an ELEMENT

Enter 3 values: the Magnet Coarse-Range (0-10) and the Magnet Interval
  (300-9700) in which you expect to find peaks: 8,

Example: 8,4330,8510

Present coarse-range=8, with 208 peak at 5564 and 207 peak at 6964.
 Interval between peaks is 200.

Use Cup and Daly, as required

"Peaks" must be >.1 mV
```

1	Cup Only	2	Larger Peaks	3	Smaller Peaks	4		5	
6		7		8		9		0	

You may need to do this part by trial and error, so don't worry if you aren't sure of the values that *Analyst* is requesting. The lower the coarse-range, the lighter the isotopes that can be included in the magnet interval. For example, Pb (masses 204 to 208) occurs at a coarse range of 8 for a high voltage of near 8 kV, Nd (masses 142 to 150) at a coarse range of 7, and Sr (masses 84 to 88) at a coarse range of 5. Also, in any coarse range, there are roughly 200 magnet units separating each mass-unit for a high voltage near 8 kV.

Before you enter the coarse-magnet range and magnet interval for the scan, you may want to over-ride the default collector used for the scan and the default minimum peak-size, by using the **F1** - **F2** - **F3** toggles. If all the peaks of interest are large, selecting **Cup Only** will speed up the scan.

To get an idea of what ballpark figures to enter for the two values requested, it might be useful to bring up several different *Elements* with the CHANGE ELEMENT key from the *bms* and look at the coarse and fine magnet values that are displayed with them. Of course, you'll need to do this before you request the NEW ELEMENT procedure.

Analyst will then do a graphics magnet-scan over the interval that you requested, with a logarithmic Y-axis (beamsize). As soon as the scan is finished, *Analyst* will indicate the first peak encountered with a large arrow on the graphics, and query,

Enter Mass, Nuclide of this peak (e.g. "88,Sr", "160,NdO", "87,Sr(Rb)")

Enter the mass-number of the peak, comma, nuclide or ionic species of the peak. Don't enter the precise atomic weight of the peak - for example, enter **206** rather than **205.973**. Note that the "NUCLIDE" can indicate any information you want, so long as you use no more than 6 characters.

The large arrow will then move and point to the next peak encountered in the scan, and ask the above question again until you have entered the mass and nuclide for each of the peaks encountered in the scan. At this point, *Analyst* will take a minute or so to find the half-peak magnet-offset for the peaks, center all of the peaks, and calculate a least-squares quadratic curve for the magnet-settings as a function of the mass of the peak.

You'll probably want your new ELEMENT to include information about peaks that weren't present during the scan, so *Analyst* will now query,

```
Specifying up to 24 Isotopes for the ELEMENT

Enter Isotope (integers only), Nuclide...

Examples:  85,Rb   160,NdO   87,Sr(Rb)

(nuclide names must have <=6 characters and no commas)

Isotope, Nuclide #12  (ENTER with no response when done):
```

Enter the mass and nuclide as before, and continue answering the query until all of the desired nuclides have been entered. Include all of the nuclides that you may want to either take data on, monitor for interferences, or just look at occasionally. No more that 24 nuclides may be defined, however, so you may need to prune your list a bit.

^{187}Re will also be included in your list of defined nuclides for the *Element* if possible. If the center filament is hot enough (more than about 4 amperes), *Analyst* will try to center the 187 peak using the magnet values stored with the Re *Element*. If the centering is successful, then the ^{187}Re peak will be accessible from the new *Element* by pressing **Page Down** from the *bms*.

Defining RUNNING DATA: -- When you've finished with the magnet- and nuclide-calibration procedure (or if you've specified **Change Running Data Only**), *Analyst* will bring a *Form* that looks something like this:

```
Reference Isotope -------------------> 144
Normalizing Isotope (0 if none)        146
146/144 Ratio for Normalization        .7219

Zeroes Above & Below each Peak (0)
  or at a specific mass (e.g. 144.32)  0

Report Data with Ref-Isotope in
 Numerator (1) or Denominator (2)      2

Is there a Double-Spike for this
  ELEMENT (Y/N; NO if not sure)        NO

#1: Monitor Isot, Interfering Isot     147,144
    Natural 144/147 Ratio              .2097
#2: Monitor Isot, Interfering Isot     147,148
    Natural 148/147 Ratio              .7478
#3: Monitor Isot, Interfering Isot     147,150
    Natural 150/147 Ratio              .4957
#4: Monitor Isot, Interfering Isot     140,142
    Natural 142/140 Ratio              .1251

Daly mass-discrimination, in %/amu     .14
Default-focus settings (name)          Default
```

Press the **F1 Help** for this *Form* to get a detailed explanation of whichever parameter the cursor is on (the above *Form* is just an example; the exact queries will depend on whether the *Element* is fractionation-normalizable or not). The **HELP** screens will tell you that:

The Reference Isotope is the isotope to which all others will be ratioed, and is important mainly for fractionation-normalizable *Elements* (you can specify any reference isotope during running for non-normalizable *Elements*). Typical reference isotopes are 86 for Sr, 144 for Nd, and 206 for Pb.

The Normalizing Isotope is the isotope whose ratio with the Reference Isotope (for the natural element) will be used to correct for isotopic fractionation during the run. Typical Reference-Isotope:Normalizing-Isotope pairs are 86:88 for Sr or 144:146 for Nd.

The Ref-Isotope/Normalizing-Isotope Ratio of Natural Element is the true (or "accepted") value of the reference/normalizing isotope ratio of the natural element -- for example, 0.1194 for $^{86}Sr/^{88}Sr$. This query will only appear if you have entered a nonzero Normalizing Isotope.

Your response to the Zeroes Above & Below each Peak or at a Specific Mass query determines where *Analyst* will take zeroes (backgrounds) during isotope-ratio data-taking. Normally, you should always enter ***0***, which specifies that zeroes be taken at offsets above and below each peak. The offsets will be the lesser of 0.5 mass-units or 0.34% of the peak's mass -- for example, at masses 205.5 and 206.5 for a peak at mass 206, and at masses 86.7 and 87.3 for a peak at mass 87. But if you expect that tailing or some funny isobaric interferences will prevent you from getting the true zeroes for your peaks (possibly true, for example, for UO_2 peaks), you can specify that zeroes be taken at a single, specific mass-position such as 232.36.

The query "*Is there a Double-Spike for this ELEMENT*" appears only for *Elements* that are not (naturally) fractionation-normalizable, such as Pb, Rb, and U. Though such elements have no naturally constant ratio that can be used for fractionation-normalization, you may be able to obtain a pair of artificially-produced isotopes

of the element and prepare a mixed-spike of these isotopes. Because the ratio in the mixed-spike is constant, you can then normalize the ratios (for such a spiked run) of the naturally-occurring isotopes to those of the mixed-spike isotopes, and obtain much more precise ratios (and concentrations). Examples of such double-spikes are 233+236 for uranium, and 202+205 for lead.

For such elements, you can define the mixed-spike ratios via the usual spike-definition routine (**Shift F7 F3** from the *bms*). When you run such a spiked element, just tell *Analyst* which spike-number you used, and the data for the run will be automatically corrected for fractionation, and the SAM/SPK ratio calculated and printed out for each block.

The response to Ref-Isotope in Numerator or Denominator? tells *Analyst* how you want your ratios reported: with the reference in the numerator (e.g. 238/235 if 238 is the reference isotope) or the denominator (e.g. 235/238). This is purely a stylistic preference, and has no affect on the data itself.

The next 8 queries deal with corrections for isobaric interferences. You can correct for up to 4 such interferences, so long as the interferences are not for a peak which itself will be used to monitor for interferences. For each interference, enter two isotopes, separated by a comma, for the Monitor Isotope, Interfering Isotope query. The Monitor Isotope is the nuclide that will be used to estimate the amount of elemental interference present; the Interfering Isotope is the nuclide that actually is being interfered with. For example, for strontium runs, one monitors the ^{85}Rb peak to correct for ^{87}Rb interference on ^{87}Sr -- so the response to the query would be **85,87**.

The Natural Interf./Monitor Ratio is the Interfering-Isotope:Monitor-Isotope ratio of the natural, interfering element, as it would be measured under typical running conditions for the *Element* being defined. In other words, the ratio that you enter should be "fractionated" to the extent that you would expect for actual running of the element of interest.

You may enter more than one interference for the same monitor isotope, as in the example above. Don't enter responses to any more isobaric interferences than you actually will have, though (just leave the single question-marks as your response).

For *Elements* that aren't fractionation-normalized, *Analyst* will now ask you to specify a mass-discrimination factor for the Daly detector. This factor, in percent per mass-unit (positive if in favor of the lighter isotopes), will be used to correct the reported isotope-ratio data. For example, a Daly mass-discrimination factor of 0.2 for Pb would mean that the measured 206/204 ratios would be corrected by multiplying by 1.004 (=1+2x0.2/100). You'll have to determine the correct mass-discrimination factor yourself - generally by bracketing blocks of Daly data with Faraday cup data and comparing the results.

The last query asks for the name of the default focus-settings (see **Focus Files** in the **F2 Focus** menu from the *bms*). If you have a preferred set of focus conditions for this *Element* and those settings are defined in the **Focus Files**, enter that name. Otherwise, just enter the word **Default**.

Analyst will then display the *Elements* that have already been defined, and request a number and name to assign to the new *Element*. Select an un-used number, unless you really want to replace an existing *Element*. You can use up to 6 characters for the name of the element. Don't create two *Elements* that differ only in the case of their characters, though, because *Analyst* will ignore any case differences.

The ELEMENT EDIT Routines: -- If you don't want to define a completely new *Element* from scratch, but rather want to re-use or modify an existing *Element* (though perhaps store under a different name), first select the *Element* that you want to edit using **F7 Change Elem.** from the *bms*, bring the ↑**F1 Magnet** menu up from the *bms*, and press **F1 Edit Element**. The screen will then show:

```
Routines to modify a previously-defined Element,
then either re-name or re-store the modified Element

F1 Modify magnet-values only
   (recalibrate for magnet or HV drift; calibrate for new HV)

F3 Modify isotopes only
   (specify different isotopes and/or nuclides)

F5 Change Running-Data only
   (redefine normalization, interferences, bkgrds, reference-peak...)
```

Select which part of the current *Element* you want to modify (remember, you must already have an ion-beam for the element of interest if you choose the **Modify magnet-values only** option). *Analyst* will run you through only the relevant part of the NEW ELEMENT procedure (described above), then ask you whether you want to store the modified *Element* under a new name, or just replace the old *Element*.

As an example of why you might want to modify an existing *Element* instead of defining a completely new *Element*, you might want to:

1) Define a samarium *Element* by keeping the magnet-calibration data for an already-defined neodymium *Element*, but redefining the nuclide names and running data;

2) Define an *Element* to run at a different high-voltage, in which case you'd need to modify the original magnet-values but not the isotopes, nuclides, or running data (remember, though, that slight drifts in the high voltage or magnet are more easily corrected by the DRIFT ADJUST procedure available from the ***Magnet*** menu);

3) Change only the normalization and reference-peak for an *Element* (for example for Nd, you might want two Nd *Elements* with one normalized to 146/144 and the other to 148/142).

Changing the Hardware Configuration

If you change something about the computer hardware or the mass-spectrometer, you may need to inform *Analyst* about the changes. To do so, press **Shift F1** from the MASS-SPEC STATUS menu (**Shift F7** from the *bms*). You can then change information in the CONFIGURE file concerning:

- Presence or absence of a Daly detector
- Presence or absence of a barrel motor
- Whether the barrel can hold 6 or 16 samples
- The maximum allowable Source-can and Flight-tube pressures for data-taking
- If a titanium-sublimation pump is installed and the TSP-inhibit bit of the multiple interface is to be used (to suppress the TSP during data taking)
- If a Solartron DVM is installed and is to be used for data taking[1]

How *Analyst* Calculates Isotope Ratios and their Errors

I've covered this subject to some degree in the **Manual Running** section, but will go over it again here in somewhat more detail.

After the appropriate background values (zeroes) have been subtracted from the raw peak heights collected during the peaktop-jumping part of the block, any calculated isobaric interferences are subtracted from the peaks. If the interference-monitor peaks were measured only before and after the peaktop-jumping, a linear interpolation of the interference-monitor peaks is used to estimate the amount of interference at the time that each interfered-with peak was measured. If the interference-monitor peaks were measured during the peaktop-jumping sequence (as is done for relatively large interferences), the size of the interference-monitor peaks is estimated for the time of each interfered-with peak by fitting a cubic polynomial to the intensities of the interference-monitor peaks with time.

The raw ratios of the isotopes are then calculated, using the linear-interpolation method of Dodson (1978), which corrects for any second-order curvature of the ion-beam with time. The effect of the time constants of the amplifier system on the ratios is then calculated, and the resulting small correction applied to the raw ratios.

If the *Element* were one that requires normalization of mass-fractionation using an internal ratio (such as Sr, Nd...), the normalizing ratio is calculated first, and a linear regression of this ratio with time is calculated. Using this regression, the amount of fractionation (using the exponential law of Russell and others, 1978) is estimated for the time of each individual set in the block. If the run were for a spiked sample and a fractionation-normalizable *Element*, *Analyst* will calculate the sample/spike ratio (specifically, the ratio of the sample reference-isotope to the spike's most-abundant isotope) and the fractionation-corrected radiogenic-isotope ratio. This calculation also assumes an exponential fractionation law.

The calculated errors for the ratios of each block are calculated from the sum of the following variances:

1) The set-to-set variance (that is, just the square of the standard deviation of the ratios of each set);

2) The background variance, calculated from either the observed background noise (long background counts) or the know dark noise of the particular collector (short background counts);

3) The variance from the isobaric-interference corrections, if any. This is calculated from a combination of the theoretical noise for the interference-monitor peaks plus the background uncertainty of the interference-monitor peaks plus as assigned 2% uncertainty in the assumed ratio of the interfering isotope/monitor isotope;

---

[1]Requires at least two user-written sub-programs: **Solar_set** to initialize the Solartron DVM, and **Solar_read(Counts)** to read the Solartron DVM. These sub-programs must exist in a file named **si7063** that is present in the main *Analyst* directory. Integration time for the Solartron must be set to 1 second.

4) The variance from the fractionation-correction (if any), calculated from the uncertainty in the normalizing ratio;

5) The theoretical variance of the ratio, as calculated from a combination of the dark noise of the collector and the counting statistics from the number of ions arriving at the collector. If the observed variance is greater that this theoretical variance, the observed variance is the one that is used; otherwise, the theoretical variance is used.

6) If the run were a spiked run of a fractionation-normalizable *Element*, the propagated uncertainties of the double-spike calculation are included in the errors of the spike-corrected ratios.

Defining or Editing Spikes

To define a new normalizable-element spike or to edit the isotope ratios of an existing spike on disk (or to just look at the isotope-ratios assigned to a particular spike), bring up the ***Spikes*** menu from the *bms* by pressing **Shift F7**. To edit or define a spike, you'll have to know:

- The ratios of two nonradiogenic-isotope pairs (3 isotopes sharing the same reference peaks) for the natural element of interest -- for example, the 88/86 and 84/86 ratios for strontium. Though one of these ratios should be whatever the "accepted" value is, the other should be the ratio that you would actually measure on the mass-spectrometer when fractionation is normalized to the first ratio.

- The ratios of these same two nonradiogenic-isotope pairs for the particular spike that you're defining. These ratios should be the ratios that you actually measure on the mass spectrometer (as opposed to what someone else says they should be), and should be corrected for isotopic fractionation as best you can.

- If the element has a radiogenic isotope (such as ^{87}Sr or ^{143}Nd, the radiogenic isotope-reference isotope ratio of the spike.

Manual Beam-Tuneup Functions

If you'd rather assume complete and specific control of the beam-tuneup, rather than rely on the automatic beam-tuneup functions of *Analyst*, you can do so from within *Analyst* rather than use the hardware controls on the mass spectrometer. These manual beam-tuneup functions are described below.

Manual Focus: -- Invoke the **Focus** menu with **Shift F2** and press **F2 Manual Focus** (or you simply press **F** during the *bms*). The beam-chart and focus graphics will appear on the screen. You can change the focus settings continuously by moving the joystick, in 1-unit increments by pressing the plus/minus keys or up/down-arrows, or in large increments with the PageUp/PageDown keys. Change the focus "plate" with the left/right arrow-keys, or by simply pressing the number-key for the "plate" of interest.

Manual Magnet-Scan: -- You can scan the magnet with the joystick or cursor keys by pressing **F4 Magnet Stick** from the **↑F1 Magnet** menu from the *bms* (or just press **J** from the *bms*). Using the function keys, you can then change the "speed" of the joystick or cursor-key response, or switch the magnet coarse-range. Screen beam-chart graphics are provided in the form of an X-Y recorder so that you can see peaks as they are encountered.

Manual Barrel-Scan: -- To rotate the barrel manually using the joystick or cursor-keys, press **F1 Manual Adjust** from the **Barrel** menu (**Shift F3** from the *bms*). Normally, *Analyst* won't let you rotate the barrel beyond the region where filament-contact can be maintained. If you want to override this protection, you must press the Shift key at the same time you change the barrel position. Note that the barrel mechanism has some free play (generally 5 to 15 barrel-units) so that to reproducibly arrive at the same physical barrel position, you'll need to approach that position from the same rotational direction each time.

Hardware Diagnostic Functions Available within *Analyst*

Several utilities for troubleshooting are available within *Analyst*. Many of these can be specified as part of the automatic running procedure (see the section on **Automatic Hardware-Diagnostic Functions** in **Automatic Running**), or invoked as a sequence in manual running from the *bms* (bring up the **Hardware** menu with **Shift F6**, then press **F4**).

Scanning the Focus Potentials: -- For troubleshooting ion-optics problems, or just for getting a feel for the effect of varying the various focus potentials, you can scan the focus potential for any "plate" and graphically see the effect on the beam. Press **F3 Scan Focus** from the **Focus** menu (**Shift F2** from the *bms*; or just press **S** from the *bms*), and then select the plate that you wish to scan and the scanning step-interval from the *Form* that follows. The *Form* also has an option that will allow you to have the DAC (digital to analog converter) output for some of the plates be the Y-axis of the scan.

You can also ask *Analyst* to scan all of the plates for both beam response and DAC response by selecting this option (press **Shift F3**) from the ***Focus*** menu (**Shift F2** from the *bms*). For DAC checks, this routine will not only show you the graphics of the scan, but will also flag apparent problems on the graphics display, and mathematically examine the output and tell you whether or not there seems to be any hardware malfunctions. If the printout says that the DAC scans indicate no problems, those DACs are probably OK. Graphics will be dumped to the printer only for scans which indicate apparent problems.

Checking the Stability of the Accelerating Voltage: -- To check the degree of drift (linear change of accelerating voltage with time) and noise (about this linear drift) of the accelerating voltage, bring up the ***Focus*** Menu (**Shift F2** from the *bms*), then press **Shift F4**. You must select the time interval over which the drift and noise are to be monitored. This is also one of the Automatic Hardware-Diagnostic Routines (**Shift F7, F4** from the *bms*). This routine will numerically evaluate the drift and tell you whether or not it falls in the normal range. If you still have questions about the stability of the accelerating voltage, you can either:

1) In manual mode, request that the HV be monitored and printed out before every data-block. Do this by invoking the ***Focus*** menu (**Shift F2** from the *bms*) and toggling with **Shift F3**. You can then invoke a graphical evaluation of the block-to-block HV drift at any time by pressing **Shift F6** from the ***Focus*** menu.

2) In automatic mode, toggle the **Show HV drift for each block within run** function of the Automatic Diagnostic Routines.

Calibrating the Time Constants of the Amplifier System: -- The time constants of the amplifier system (mostly arising from the 10^{11} ohm resistor) determine how much apparent beam remains at a given number of seconds after the magnet has shifted from a peak to a zero-position. Because *Analyst* corrects the raw data for this "memory" effect, these time constants should be recalibrated at least twice a year. To invoke the calibration routine (which requires a 5-volt, stable ion-beam), bring up the **Hardware** menu from the *bms* (**Shift F6**), then press **F10** (or simply press **Ctrl T** from the *bms*).

Graphics Pressure-Monitor: -- To use the computer as a logarithmic stripchart-recorder for the pressure in both the source can and the flight tube, press **F2 Pressure Graph** from the **Hardware** menu (**Shift F6** from the *bms*) -- or simply press **Ctrl G** from the *bms*. You can then define the time-interval of the chart, the maximum pressure to be shown, and whether or not to dump the chart to the printer each time it reaches the time-interval.

Checking Abundance-Sensitivity and Resolution: -- If you have a beam of 2 volts or more arriving at the collector, you can invoke a scan to check the abundance-sensitivity and resolution of the mass spectrometer by pressing **F9** from the **Magnet** menu (**Shift F1** from the *bms*) -- or simply press **Ctrl A** from the *bms*. *Analyst* will scan from a mass-unit or so below the peak you were on when you invoked this routine, up to the half-mass above that peak.

The scan will be done using the Daly (except, of course, as large peaks are encountered) and displayed using a logarithmic scale of beam-size versus magnet-position. The graphics will also show the expected beam-tail for the factory-specified abundance sensitivity (10 ppm tail at 4200 ppm of mass below a peak, at a flight-tube pressure of $1\text{-}2\times10^{-8}$) and how much tail was actually observed (you should get <3 ppm for a $<2\times10^{-9}$ flight-tube pressure). The abundance-sensitivity directly reflects, among other factors, the flight-tube pressure, so don't expect to meet the factory specs if the flight-tube pressure is much greater than the above value. The resolution indicated by the graphics should be at least 370 or so, and no better than about 420 unless you have decided to sacrifice beamsize for resolution by narrowing the collector slit.

Hall Probe Check: -- To check the functioning of the Hall probe and also the magnet, you can invoke the *Hall Probe Check* routine from the ***Magnet*** menu (**Shift F1** from the *bms*) by pressing **Shift F1**. This function will graphically show the Hall-probe output as a function of magnet-setting for a scan over an arbitrary range. The graphics should show a smooth, monotonic, and constant-slope response (except for 1-pixel jumps, of course) of the Hall-probe output with magnet-setting. *Analyst* will mathematically evaluate the smoothness of the response (as well as graphically flag any problem areas), and tell you whether there is any apparent problem.

Taking Collector Zeroes: -- Normally, *Analyst* only takes collector zeroes when changing samples (and for ratio-taking, but these zeroes are used only for that particular block of data). If you want to re-check the zeroes (perhaps due to a pressure rise or change in the hardware zero-settings), you can do this by pressing **F2 New Zeroes** from the **Daly** menu (**Shift F4** from the *bms*; or just press **Z** from the *bms*). ***Analyst*** will search for the magnet-position with the lowest apparent beamsize, and take zeroes for both collectors.

Rough Calibration of the Daly Gain: -- The Daly gain will vary significantly (10-30%) from element to element, or even over a time interval of a few weeks. To quickly calibrate the gain, so that the apparent Daly beamsize exactly matches the Faraday Cup beamsize, you will need to invoke the **Calibrate Daly Gain** function.

First, get a beam of between 5 and 45 millivolts. Then, press **F3 DalyCal** from the **Daly** menu (**Shift F4** from the *bms* -- or just press **Alt D** from the *bms*). *Analyst* will then center the peak, take fresh collector zeroes, and determine the current Daly gain by monitoring the peak on the Cup, Daly, then Cup again.

Calibrating the Daly Nonlinearity: -- The gain of the Daly detector is not necessarily linear with beam size, so for the most precise data you should calibrate this nonlinearity from time to time. *Analyst* can correct for a Daly nonlinearity of the form

True Beam = (Apparent Beam)[1+k(Apparent Beam)]

where **k** is the nonlinearity constant. There is no really easy way of determining **k**, but one method is to:

1) Prepare a filament-load with 3 nuclides, 2 of which are in nearly equal abundance, and the third lower by a factor of 3 to 100. For example, with U-233/U-236=1 and U-233/U-238=10.

2) Set the nonlinearity constant to **0** by pressing **F8 Daly Nonlin** from the **Daly** menu.

3) Take isotope-ratio data with one of the higher-abundance nuclides as the reference isotope, over a range of ion-beam intensities (for the highest-abundance nuclide) of 2 to 40 millivolts or so;

4) Normalize the ratios (for linear or pseudolinear mass discrimination) of the lowest-abundance nuclide to the highest-abundance nuclide using the known ratio of the higher-abundance nuclides;

5) Regress the normalized ratios against the ion-beam intensity of the highest-abundance nuclide, using an algorithm that weights the points according to the inverse of their analytical variance;

6) Calculate the nonlinearity constant with the expression

$$k = \frac{SR_m}{R_t(1 - R_m)}$$

where k is the nonlinearity constant, S is the slope of the regression line, R_m is the measured (but corrected for mass discrimination) ratio, and R_t is the true ratio. You can use the intercept of the regression line to estimate R_t;

7) Inform *Analyst* of this value from the *Daly* menu (**Shift F4** from the *bms*) by pressing **F8 Daly Nonlin.**

Checking the Degree of Peaktop Flatness: -- The quick peak-shape check (**F3** from the Magnet Menu or **P** directly from the *bms*) will give you a quick (takes about 15 seconds) visual and semi-quantitative idea of the width of the flat-topped part of the peak, and tell you whether or not the peak is grossly non-flat. This check can be invoked as part of the auto-run diagnostics, in which case the check will be run before each block on the largest data-collecting peak, using the data-taking collector (only numerical results will be printed out).

For the highest-quality data, however (run-to-run precisions of better than 100 ppm), the peak must be flat to a much greater degree than the quick graphics peakshape can tell you. To do a precise check of the peak flatness, you will need a stable beam of at least 2 volts (Cup) or 10 millivolts (Daly).

Invoke the quantitative peak-flat check by pressing **F8** from the Magnet Menu (or just press the ~ key directly from the *bms*). The resulting *Form* will ask you to select the isotope for the check, the collector (Cup or Daly), the beam-size to be used, the number of ratios, and the magnet offset-step. The peak-flat check will determine the ratios of the peak-height at each of 6 offsets (from the center of the peak) to the peak-height at the center of the peak. The offsets will be at -3, -2, -1, +1, +2+ and +3 steps from the center of the peak, where the step size is the "magnet offset-step" value referred to above. The "magnet offset-step value" is in ppm of the mass of the isotope being used: typical regions of peak flatness are about 500 ppm of mass.

The results will be displayed in terms of the difference between the peak-height at each offset and the peak-height at the center of the peak, in ppm. To get a precision on these values of 10 to 20 ppm, you will need on the order of 100 ratios (takes ~15 minutes). When the check is complete, *Analyst* will give you a graphical display of the results and dump the display to the printer. The peak should be flat to within 100 ppm over a width of 500 ppm of mass for the Cup, or to within 1000 ppm over 300 ppm of mass for the Daly.

The quantitative peak-flat check can also be invoked either at the end of a sequence of automatic runs, or at the end of each automatic run, as part of the auto-run diagnostics.

Checking for Magnet Drift During a Run: -- At the end of each automatic run with more than 3 blocks, *Analyst* will examine the magnet-settings for the **MIP** against the time of centering. If the magnet drift or scatter is excessive, graphics with a plot of the magnet-settings versus time will be dumped to the printer. You can also request this procedure from the *bms* at any time for the current run by invoking the Magnet Menu (**Shift F1**), then pressing **Shift F3**. A message of excessive scatter or drift indicates a problem with either magnet electronics or accelerating-voltage stability (or possibly just a very noisy ion-beam).

Checking for Background Drift During a Run: -- At the end of each automatic run with more than 3 blocks, *Analyst* will examine the background-readings for the **MIP** against the time of the block. You can also request this procedure from the *bms* at any time for the current run by invoking the Collectors Menu (**Shift F4**), then pressing **F6**. The backgrounds (especially Daly Detector backgrounds) are affected by the beam-size and by the flight-tube pressure, so some variation is normal.

Checking for Accelerating Voltage Drift during a Run: -- At the end of each automatic run with more than 3 blocks, *Analyst* will examine the accelerating voltage at the beginning of each block against the time of the block. If the drift or scatter in accelerating voltage is excessive, graphics with a plot of the accelerating voltage versus time will be dumped to the printer. You can also request this procedure by invoking the ***Focus*** Menu (**Shift F2**), then pressing **Shift F6**. A message of excessive scatter or drift indicates a problem with accelerating-voltage stability.

Checking for Pressure Drift during a Run: -- *Analyst* keeps track of the source-can and flight-tube pressures measured at the start of each block for each run. To force graphs of pressures versus time to be dumped after each automatic run, invoke press **Shift-F6 F4 Aut Diagnostic** from the *bms* and specify pressure-graph dumps. To have a quick look at trends for pressures during or just after any run, press **Shift-F5 F4 Pressure Drifts** from the *bms*.

Graphics Monitoring of Miscellaneous Device Outputs: -- You can use the screen as a real-time graphics monitor of any of the mass-spectrometer devices that can by queried by the computer by pressing **Shift F2** from the MASS-SPEC STATUS menu (**Shift F7** from the *bms*). The display will be:

```
Ion Gauge
Pirani
Ion Pump 1
Ion Pump 2
Digital Integrator Zero
Magnet Current
D-Focus (4)
Z-Focus (6)
Extraction (2)
Slit (5)
Hall Probe
High Voltage
FA3 (Daly output)
Faraday Cup output
Sample-Filament Flag
Preheat-Filament Flag
```

Pick a device to monitor by moving the cursor-bar. *Analyst* will then ask you to set up the graphics limits, and begin monitoring.

Idle Time Diagnostics: -- If, between the hours of 1 A.M. and 6 A.M., *Analyst* finds itself idle (that is, in the *bms* without any recent operator interaction) for more than an hour or so, the following hardware-diagnostic routines will be run, and their results dumped to the printer: focus-DAC scans, Hall-probe output scan, and accelerating-voltage stability-test.

Miscellaneous Other Functions Available from *Analyst*

Defining and Using Default Focus-Values: When *Analyst* rotates a new sample into running position, and when the *Element* is changed (if the filament-currents are off), the focus-settings are restored to the default focus-settings specified in the current *Element*'s definition. In most cases, the "Default Single" or "Default Triple" settings are adequate (though after a change of sources, these settings should also be changed to reflect the slightly different physical configurations of different sources). For some types of runs on particular elements, though, different focus-settings may yield better beams, in which case you may want to define an *Element* with specific, non-standard focus-settings (that is, a different *Default Focus*). If both the *Element* and *Default Focus* already exist, you can change its *Default Focus* by selecting **Edit Element** from the Magnet Menu (**Shift F1** from the *bms*), and specifying **Run-Data Only**. The *Default Focus* settings are also used when *Analyst* is first instructed to focus on a very small or absent ion-beam for a sample. If no beam is detected using the *Elements* default focus-settings, *Analyst* will try each of the defined Default Focus settings for that type of filament (single or triple), in the order they appear in the list of such settings. Only if none of the Default Focus settings yields a beam will *Analyst* revert to the highest-priority, Default-Single or Default-Triple settings, and scan each "plate" over its full range to try and find a beam.

To access the *Focus Files*, press **F5 Focus Files** from the **Focus** menu (**Shift F2** from the *bms*). From the resulting Focus File Screen you can:

1) Define settings for a completely new Default Focus by typing in the new settings (**F2**);

2) Define the current focus positions as one of the Default Focus settings (**F3**);

3) Change the order (priority) that the defined Default Focus settings are invoked when trying to focus an extremely small beam (**F4**);

4) Specify whether to edit Default Focus settings for single-filament or triple-filament samples (**F5**);

5) Modify any of the defined Default Focus settings (**F6**); or

6) Delete a Default Focus setting (**F7**).

Note that *Analyst* may independently change the Default Focus settings from time to time. This will happen if the gain in beamsize for the first focus of a sample exceeds about 20 for three consecutive runs. In this case, the final focus-settings for the third run will be used (and stored on disk) as the default focus-settings for the present number of filaments (single or triple), and a message saying so will be printed out on the printer.

Changing the Standard HV for Several *Elements*: -- If the High Voltage has drifted so that, when a new *Element* is invoked, *Analyst* is no longer on the correct peaks, it may be necessary to re-define the default High Voltage values for the *Elements*. To do this, you must first determine what the new High Voltage value should be with the following procedure: Invoke a new *Element* in the usual way (**F8** from the *bms*). Then, without attempting to center the peak, manually adjust the High Voltage from the mass-spectrometer panel until you are on top of the correct peak. Query the High Voltage from the computer (Ctrl V from the *bms*) and write down the value. Now invoke the ***Focus*** Menu (**Shift F2**) and choose the CHANGE STANDARD HV option (**Shift F1**). *Analyst* will then instruct you how to change the old High Voltage values required by each defined *Element* to the new value.

Adjusting the *Element* Magnet-Values for Drift: -- If, when you request that a new *Element* be used by *Analyst*, you find that even though the high-voltage is at the correct value, all of the peaks are significantly off the default magnet-settings (that is, you're not on the peak-tops), you can request a quick recalibration and correction for this drift from the stored magnet-values, and re-store the corrected magnet-values for that *Element*.

To do this, you must (1) have a stable high-voltage (so the high-voltage unit must have been turned on for at least a half-hour), (2) have a stable magnet (ditto above), and (3) have at least one peak of a known isotope of significant intensity (at least a few millivolts).

Invoke the procedure by pressing **F5 Drift Adjust** from the ***Magnet*** menu (**Shift F1** from the *bms*; or just press **M** from the *bms*). If the magnet-settings are only slightly off (that is, you could center the peak with **F1 Center Peak** from the *bms*), use the AUTO option; otherwise select the MANUAL option. The AUTO option will simply try to center the peak that you were on when you invoked the procedure, and if successful, store the recalibrated values (for all of the peaks of this *Element*) on disk. The MANUAL option will require you to manually scan the magnet (using the joystick or cursor keys) until the screen graphics show that you are on a peak. After you identify the peak, *Analyst* will center it and recalibrate as above. In both cases, if the center-filament current is more than about 4.4 amps, the routine will try to recalibrate the ^{187}Re peak as well.

Flagging *Elements* Whose Magnet-Settings Are No Longer Valid: If you make a hardware change to the mass spectrometer (such as moving the magnet) that changes the default magnet settings for the peaks enough to prohibit centering on the correct peaks, you'll need to perform either a simple drift-adjust (**Shift F1 F5** from the *bms*) or a

complete magnet-recalibration for that *Element* (**Shift F1 F1** from the *bms*). Because all of the other defined *Elements* will be similarly affected and it may not be convenient to immediately perform a drift-adjust on them all, *Analyst* has a provision for "flagging" the *Elements* in need of such attention.

To post or remove a drift-adjust flag for one or more *Elements*, press **Shift F1 F10** from the *bms*, then select the *Elements* of interest. Once a drift-adjust flag is posted for an *Element*, it will appear with an asterisk in the list of defined *Elements*. *Analyst* will abort any automatic runs for flagged *Elements* just before trying to tune up the ion-beam for the run; you will get several warnings before this happens, though. To remove the flag, request either a simple drift-adjust or a complete magnet-recalibration for that *Element* (or use the procedure outlined above).

Executing DOS Commands from *Analyst*: You can execute any legal DOS command or short DOS program from within *Analyst* (for example, to copy or delete files or to look at file directories). From the *bms*, press **Shift F3** to bring up the **VIEW** menu, then **Shift F3** -- or just press **Ctrl E**(xecute). Note, however, that only 64 kilobytes are reserved for executing the DOS command or program.

Checking Program Version and Memory Available: To see the version number of *Analyst*, DOS, and HTBasic, press **V** from the *bms*. The amount of memory available to *Analyst* will also be shown.

Running Neodymium Samples as NdO^+

If you run neodymium as NdO^+, taking data on either (unspiked) $^{143}Nd^{16}O$-$^{144}Nd^{16}O$-$^{146}Nd^{16}O$ or on (spiked) $^{143}Nd^{16}O$-$^{144}Nd^{16}O$-$^{146}Nd^{16}O$-$^{150}Nd^{16}O$ (that is, on masses 159-160-162 or 159-160-162-166), *Analyst* will make the ^{18}O-^{17}O corrections for you. Specify the oxygen isotope ratios and neodymium isotope ratios for correction from the **Shift F8 Data** menu by pressing **Shift-F2: Specify NdO factors** (or simply **Ctrl O** from the *bms*). At the end of each NdO^+ data-block, *Analyst* will calculate the Nd metal isotope ratios by subtracting the oxide interferences. *Analyst* will also make the appropriate NdO corrections on mass 163 ($^{147}Sm^{16}O$ + $^{146}Nd^{17}O$ + $^{145}Nd^{18}O$) peak before subtracting the $Sm^{16}O$ contributions to the 160 and 166 peaks. You must, of course, define the NdO *Element* to monitor mass 163 and to correct (using the Sm metal abundances) the 160 and 166 peaks. Note that in defining the NdO *Element*, you must specify a reference isotope of 160, a normalizing isotope of 162, and a 160/162 normalizing ratio that includes the ^{17}O and ^{18}O interferences - thus

$$\frac{162}{160} = \frac{\frac{146}{144} + \frac{145}{144}R_{17} + R_{18}}{1 + \frac{143}{144}R_{17} + \frac{142}{144}R_{18}}$$

where R_{17} and R_{18} refer to the expected $^{17}O/^{16}O$ and $^{18}O/^{16}O$ ratios, respectively, and the $^{146}Nd/^{144}Nd$ ratio is the value you would normalize to for Nd^+ runs.

If the sample is spiked with an ^{150}Nd spike and you want to take data on masses 159, 160, 162, and 166, you must specify a spike with the *metal* isotope ratios (143/144, 146/144, and 150/144). So you would use the *same* 143-144-146-150 spike file for the oxide run as for the metal run.

Alphabetical Listing of Functions and Keystrokes to Invoke

Note: in the table below, the up-arrow symbol (↑) is used to indicate that the Shift key is to be depressed before the key following; for example, **↑F4 F3** indicates that **Shift F4** is to be pressed, followed by **unshifted F3**. Where more than one way of accessing the function exists, both are given, separated by commas.

This is essentially the same index that you can access from the *bms* by pressing the **?** key.

Function	Keystrokes to invoke (from bms)
Abundance-sensitivity & resolution, scan & check	CTL-A, SHFT-F1 F9
Accelerating voltage -- see High Voltage	
Adjust current *Element*'s magnet values for drift	M, SHFT-F1 F5
Age, model, Nd, calculate	CTL-N
Age, model, Pb, calculate	CTL-P
Age, model, Sr, calculate	CTL-S
Age, radiogenic Pb-207/206, calculate	=
Analyst, quit and return to DOS	SHFT-F5 F9
Analyst, version of	V
Auto-running, begin or invoke procedures for	F9
Automatic diagnostic routines	SHFT-F6 F4
Automatic running, resume from manual	Home, Backspace
Automatic running, start at an arbitrary run	SHFT-Home
Automatic-run variables, define/manipulate	SHFT-F9
Averages (weighted) of auto runs, print out	SHFT-R, SHFT-F8 F4
Averages (weighted) of run-data, calculate	A or SHFT-F8 F5
Background, jump to	< >
Background position for data-taking, change	SHFT-F8 F10,SHFT-F4 F5
Barrel, display names of samples in	N, SHFT-F3 F6
Barrel, optimize position of for best beam (auto)	F3
Barrel positions for filament contacts, display	SHFT-F3 F9
Barrel, rotate manually with Stick	SHFT-F3 F1
Barrel, store last contact-position calibr. on disk	SHFT-F3 F8
Barrel, test of filament-contacts for samples in	B or SHFT-F3 F2
Barrel-center, specify safety zones for	SHFT-F3 F4
Barrel-center, inhibit for auto-runs	SHFT-F3 F10
Beam chart, eXpanded-scale toggle	X
Beam chart, increase/decrease headroom (y-axis)	u/d (unshifted)
Beam chart, increase/decrease time-axis	SHFT U/D
Beam chart, Large/small size toggle	L
Beam chart, loG/linear Y-scale toggle	G
Beam noise & decay, toggle BMS display of	SHFT-F12
Beam tune-up, complete (center/focus/barrel/center)	Tab
Blank-out screen with screen-saver	CTL-B or Q
Bug reports, post in message-file	w, SHFT-F5 F7
Calculate a 207/206 age for Pb-isotope ratios	=
Calculate a Model-Nd age	CTL-N
Calculate a Model-Sr age	CTL-S

Calculate a Pb-isotope Model Age and μ . . . . . CTL-P
Calibrate Daly gain . . . . . ALT-D, SHFT-F4 F3
Center barrel -- see Barrel-center
Center peak (by changing magnet) F1
Center-filament, change current of (if enabled) . . . . . CTL-Stick, F5
Change *Element* F7
Change sample (reset barrel first) F8
Change sample (quick, no barrel-reset) . . . . . Alt C
Collector zeroes, measure . . . . . Z, SHFT-F4 F2
Collimator -- see FOCUS
Complaints -- Surely you jest! . . . . . w, SHFT-F5 F7
Configuration of hardware, change . . . . . SHFT-F6 F8, H
Contact test for all samples in barrel . . . . . B or SHFT-F6 F7
Contacts for sample being run, check . . . . . CTL-F or SHFT-F6 F6
D-focus output, graphics monitor of . . . . . SHFT-F6 F9, ALT-G
Daly Enable/Disable status, change . . . . . CTL-D, SHFT-F4 F4
Daly gain, calibrate . . . . . ALT-D, SHFT-F4 F3
Daly gain, specify SHFT-F4 F7
Daly, nonlinearity term, enter SHFT-F4 F8
Daly, switch to from Faraday Cup F4
Data for a run, locate on disk . . . . . CTL-L or SHFT-F8 F6
Data for the current run, transfer immediately to a RUN*nnn*.DAT file . . . . . SHFT-F8 F7 or Alt T
Data for runs, print/show . . . . . r, SHFT-F8 F3
Data-taking, manual, begin F10
Date, set . . . . . T, SHFT-F6 F5
Default focus-settings, examine files of SHFT-F2 F5
Default focus-settings, restore SHFT-F2 F5
Define a completely new *Element* SHFT-F1 F6
Define a new spike SHFT-F7 F3
Delay/integration times, manual data-taking, specify F10
Delete a Spike from disk SHFT-F7 F4
Delete an *Element* from disk SHFT-F1 F7
Deleting a Standard Run . . . . . SHFT-F9 SHFT-D
Deleting an automatic run . . . . . SHFT-F9 d
Diagnostic routines, automatic SHFT-F6 F4
Diagnostics of focus-unit, complete . . . . . SHFT-F2 F10, ALT-F
Digital Integrator Zero output, graphics monitor of . . . . . SHFT-F6 F9, ALT-G
Disable Daly-detector . . . . . CTL-D, SHFT-F4 F4
Display (=screen), last accessed, retrieve from disk . . . . . ALT Enter
Display (=screen), retrieve from disk . . . . . Enter, SHFT-F5 F10
Display (=screen), store on disk . . . . . CTL Enter
DOS, execute command from within *Analyst* . . . . . SHFT-F5 SHFT-F3, CTL-E
DOS, quit *Analyst* and return to SHFT-F5 F9
DOS, shell out to (return with EXIT) . . . . . CTL End, SHFT-F5 F8
Drift adjust for an *Element*, perform . . . . . M, SHFT-F1 F5
Drift, magnet, during last run, show/evaluate SHFT-F1 SHFT-F2
Drift, block-zeroes, show for current run SHFT-F4 F6, SHFT-F5 F5
Drift, high-voltage, show for current run SHFT-F2 SHFT-F4
Drift-adjust Flag for *Element*, post or remove SHFT-F1 F10

Dump screen to printer . . . . . CTL-PrntScrn
Element, adjust magnet-values for drift . . . . . M, SHFT-F1 F5
Element, change F7
Element, define a completely new SHFT-F1 F6
Element, delete from disk SHFT-F1 F7
Element, display parameters defining SHFT-F1 F2
Element, edit or change values for SHFT-F1 F1
Element, post or remove Drift-Adjust flag for SHFT-F1 F10
Element, re-check disk for data of . . . . . CTRL-C
Elements, change std high-voltage values for several SHFT-F2 SHFT-F1
Emulation mode, switch to/from, configure . . . . . SHFT-F6 SHFT-F5, ALT-E
Enable Daly-detector . . . . . CTL-D, SHFT-F4 F4
Enable filament-current change . . . . . * or Stick-Button
End *Analyst*, return to DOS SHFT-F5 F9
Enter sample-names for a barrel . . . . . E or SHFT-F8 F2
Error message, enter by user . . . . . w, SHFT-F5 F7
Error messages, access log of SHFT-W,SHFT-F5 F6
Execute a DOS command . . . . . SHFT-F5 SHFT-F3, CTL-E
Exit auto-running temporarily . . . . . F1 →Manual
Expanded-scale beam-chart toggle X
Extraction-plate (focus) output, graphics monitor of . . . . . SHFT-F6 F9, Alt G
FA3 amplifier output, graphical monitor of . . . . . SHFT-F6 F9, ALT-G
Faraday Cup, switch to from Daly F4
Filament contact test for all samples in barrel . . . . . B or SHFT-F3 F2
Filament contacts for current sample, check . . . . . CTL-F or SHFT-F6 F6
Filament-current change, automatic F5
Filament-current change, enable . . . . . Stick button, *
Filament-current change using Stick (when enabled) . . . . . Stick U/D
Filament-current, increase/decrease (when enabled) . . . . . U/D Arrows
Filament-current, turn off (preheat-center) . . . . . 3 (twice)
Filament-current, turn off (preheat-side) . . . . . 4 (twice)
Filament-current, turn off (sample-center) . . . . . 1 (twice)
Filament-current, turn off (sample-side) . . . . . 2 (twice)
Filament-current, turn off for ALL filaments . . . . . 5 (twice)
Filament-flags (contacts) of sample being run, check . . . . . CTL-F or SHFT-F6 F6
Filament#, change (when enabled) . . . . . L/R arrows
Find run-data on disk . . . . . CTL-L or SHFT-F8 F6
First-block normalization, changing during a run SHFT-F8 F9
Flag, Drift-Adjust for *Element*, post or remove SHFT-F1 F5
Flight-tube pressure, query . . . . . CTL-X, SHFT-F6 F1
Focus ion-optics (automatic) F2
Focus ion-optics, using Stick . . . . . F, SHFT-F2 F2
Focus potentials, graphical monitor of DAC output . . . . . SHFT-F6 F9, ALT-G
Focus settings, default, change priorities of SHFT-F2 F5
Focus settings, default, examine/edit file of SHFT-F2 F5
Focus unit, complete hardware diagnostics of . . . . . SHFT-F2 F10, ALT-F
Focus unit, scan potentials of . . . . . S, SHFT-F2 F3
Focus values, display on screen SHFT-F2 F4
Focus values, restore default SHFT-F2 F5

Focus-values, type in new SHFT-F2 F8
Full-screen beam-chart, toggle L
Daly, calibrate . . . . . ALT-D, SHFT-F4 F3
Gain, Daly, specify SHFT-F4 F7
Graphics -- see SCREEN, or specific function...
Half-peak position, jump to . . . . . [or]
Hall-Probe, graphics scan over any range F6
Hall-Probe, graphics troubleshooting of . . . . . F6 or SHFT-F1 SHFT-F1
Hardware configuration, change . . . . . SHFT-F6 F8, H
HELP (keystroke index) . . . . . ? or /
High voltage, before-block printout toggle SHFT-F2 SHFT-F3
High voltage output, continuous graphical monitor of . . . . . SHFT-F6 F9, ALT-G
High voltage, show drift of for current run SHFT-F2 SHFT-F4
High voltage, single query . . . . . CTL-V or SHFT-F2 F7
High-Voltage, change std values for several *Elements* SHFT-F2 SHFT-F1
High-Voltage, check of stability SHFT-F2 SHFT-F2
Increment run-number SHFT-F8 F8
Index, keystroke, to all of *Analyst*'s functions . . . . . ? or /
Index, keystroke, to common BMS-defined functions . . . . . ? or /
Index, keystroke, to shortcut keys . . . . . ? or /
Integration time on beam (BMS), change to 0.2 seconds . . . . . Esc
Integration time on beam, (BMS) change to 1 second . . . . . CTL * (keypad only)
Integration/delay times, manual data-taking, specify F10
Ion gauge, output of, graphics monitor SHFT-F6 F2
Ion Optics -- see FOCUS
Ion pump output, graphics monitor of . . . . . SHFT-F6 F9, ALT-G
Isotope-ratio data for runs, display/print . . . . . R, SHFT-F8 F4
Isotope-ratio data-taking, manual, begin F10
Joystick -- see STICK
Jump DOWN n masses . . . . . CTL-ALT-Fn
Jump DOWN to next-defined peak . . . . . -
Jump FROM Rhenium-187 peak to previous peak . . . . . PageUp
Jump to background . . . . . < or >
Jump to current peak-top . . . . . space-bar
Jump to half-peak . . . . . [or]
Jump TO Rhenium-187 peak . . . . . PageDown
Jump UP n masses . . . . . CTL-Fn
Jump UP to next defined peak . . . . . +
Keystroke index . . . . . K or ? or /
Lead-isotope Model-Age and μ, calculate . . . . . P
Lead-isotope radiogenic 207/206 age, calculate . . . . . =
Linearity term, Daly, specify SHFT-F4 F8
List functions of common Non-Function-key actions from BMS . . . . . K
Locate run-data on disk . . . . . CTL-L or SHFT-F8 F6
Log/Linear beam-chart, toggle . . . . . G
Magnet, adjust for peak-center F1
Magnet and *Element* data, display on CRT SHFT-F1 F2
Magnet current output, graphical monitor of . . . . . SHFT-F6 F9, ALT-G
Magnet Drift for current run, show SHFT-F1 SHFT-F2

Magnet scan, auto, do within automatic runs SHFT-F6 F4
Magnet scan, from BMS with keyboard . . . . . CTL,SHFT,ALT L/R arrow
Magnet scan from BMS with Stick . . . . . Stick L/R
Magnet scan, semi-automatic F6
Magnet scan using Stick with beam as Y-axis . . . . . J, SHFT-F1 F4
Magnet scan with Hall-Probe output as Y-axis F6
Magnet, switch to different peak -- see PEAK-JUMP
Magnet values, adjust for HV- or magnet-drift . . . . . M, SHFT-F1 F5
Magnet values during last run, show/evaluate SHFT-F1 SHFT-F2
Manual barrel-rotation with Stick SHFT-F3 F1
Manual data-taking, begin F10
Manual ion-optics focusing . . . . . F or SHFT-F2 F2
Manual magnet scan using Stick, w. graphics . . . . . J, SHFT-F1 F4
Manual magnet-scan from BMS (joystick) . . . . . Stick L/R
Manual magnet-scan from BMS (keyboard) . . . . . CTL,SHFT,ALT L/R arrow
Means, weighted, of run-data, calculate . . . . . A or SHFT-F8 F5
Memory, available to *Analyst* V
Message, post in user message-file . . . . . w, SHFT-F5 F7
Messages (warning or user), access log of SHFT-W,SHFT-F5 F6
Model age, Nd, calculate . . . . . CTL-N
Model age, Pb, calculate . . . . . CTL-P
Model age, Sr, calculate . . . . . CTL-S
Name of sample for current run, change in mid-run SHFT-F8 F9
Names of samples in barrel, display list of . . . . . N, SHFT-F3 F6
Names of samples in barrel, Enter or Edit . . . . . E, SHFT-F3 F5
Neodymium oxide runs, specifying correction factors for . . . . . SHFT-F8 SHFT F2, CTL O
Neodymium model-age, calculate . . . . . CTL-N
Noise, beam, toggle BMS display of SHFT-F12
Non-Function-key functions defined during BMS, list of . . . . . K
Nonlinearity term, Daly, enter SHFT-F4 F8
Normalization to first block, changing during run SHFT-F8 F9
Overview (wtd averages) of auto-runs, print out . . . . . SHFT-R or SHFT-F8 F4
Oxide correction factors for NdO runs, specifying . . . . . SHFT F8 SHFT F2, CTRL O
Pause program . . . . . CTL-Backspace
Pb-isotope model-age and μ, calculate . . . . . CTL-P
Pb-isotope radiogenic 207/206 age, calculate . . . . . =
Peak center (using magnet) F1
Peak-flat check, auto, after every automatic run SHFT-F6 F4
Peak-flat check, quantitative, single check . . . . . ~, SHFT-F1 F8
Peak-flat check, quick, graphical only . . . . . P or SHFT-F1 F3
Peak-jump, down 1 of n masses . . . . . - or CTRL-ALT-Fn
Peak-jump, up 1 or n masses . . . . . + or CTRL-Fn
Peak-scan (magnet), manual F6
Peak-scan, magnet, auto, do within auto-runs SHFT-F6 F4
Peak-scan, magnet, do at end of each auto-run SHFT-F6 F4
Peak-shape: see Peak-flat
Peak-side, jump to . . . . . [or]
Peak-top, jump to . . . . . Space Bar
Pirani gauge, output of, graphics monitor . . . . . SHFT-F6 F9, ALT-G

Post message in user message-file ..... w, SHFT-F5 F7
Post/remove drift-adjust "flag" for *Elements* SHFT-F1 F10
Pressure, add calibr. point to existing calibr. file ..... %, SHFT-F6 SHFT-F1
Pressure, calibrate using calibr.-point file SHFT-F6 SHFT-F3
Pressure, continuous graphical monitor of ..... CTL-G or SHFT-F6 F2
Pressure, erase old calibr. file and start new SHFT-F6 SHFT-F2
Pressure, show calibr.-point file SHFT-F6 SHFT-F4
Pressure, single query of ..... CTL-X or SHFT-F6 F1
Printout isotope-ratio data for runs ..... r or SHFT-F8 F3
Printout results of wtd avg calcs for auto-runs ..... SHFT-R, SHFT-F8 F4
Printout Run Variables ..... SHFT-F9 p
Printout Standard-Run Variables ..... SHFT-F9 SHFT-P
Program, pause ..... CTL-Backspace
QA documentation printout (revision date...) ..... SHFT End
Query accelerating voltage SHFT-F6 F3
Query pressure of source-can and flight-tube SHFT-F6 F1
Quit *Analyst* (return to DOS) SHFT-F5 F9
Re-enter auto running at the start of any run ..... SHFT-Home
Re-enter auto running (after temporary exit), same run ..... Home, Backspace
Re-start *Analyst* from scratch (power-on state) ..... CTL-Del
Resistor time-constants, measure ..... CTL-T, SHFT-F6 F10
Resolution and abundance-sensitivity, scan & check ..... CTL-A, SHFT-F1 F9
Restore default focus values SHFT-F2 F5
Restore full *bms* screen (toggle beam-graphics) ..... Esc
Resume auto-running after reversion to manual ..... Home, Backspace
Revert to manual running from auto-running ..... F1 →Manual
Revision date & author, for QA documentation ..... SHFT End
Revision date of *Analyst*, display V
Rhenium-187 peak, jump to ..... PageDown
Rotate barrel -- see Barrel
Run data, disk files, examine/locate ..... CTL-L or SHFT-F8 F6
Run data, print/show ..... r, SHFT-F8 F3
Run Number, increment without changing sample SHFT-F8 F8
Run Overview (wtd averages of auto-runs), print out ..... SHFT-R, SHFT-F8 F4
Run Variables, defining/editing/viewing SHFT-F9
Safety zones, for barrel-center, specify SHFT-F3 F4
Sample, change (reset barrel first) F8
Sample, quick-change (no barrel-reset) ..... ALT-C
Sample names for barrel, display ..... N or SHFT-F3 F6
Sample names for barrel, enter ..... E or SHFT-F3 F5
Scan focus-potentials or DAC outputs ..... S, SHFT-F2 F3
Scan magnet, do at end of each auto-run SHFT-F6 F4
Scan magnet, do within automatic runs SHFT-F6 F4
Scan magnet semi-automatically, beam or Hall-Probe F6
Scan magnet using joystick or cursor keys ..... J, SHFT-F1 F4
Screen blanker, invoke ..... CTL-B, Q, q
Screen, dump to printer ..... CTL PrintScrn
Screen image, any, retrieve from disk ..... Enter, SHFT-F5 F10
Screen image, last accessed, retrieve from disk ..... ALT Enter

Screen image, store on disk . . . . . CTL Enter
Set Time and/or Date . . . . . T, SHFT-F6 F5
Shell out to DOS (return with EXIT) . . . . . CTL End, SHFT-F5 F8
Shifted-function-key menu, restore . . . . . Esc
Side-filaments, change current of (if enabled) . . . . . Stick, U/D arrows, F5
Slit-plate (focus) output, graphics monitor of . . . . . SHFT-F6 F9, ALT-G
Solartron DVM, initialize . . . . . SHFT-F6 SHFT-F6, ALT-S
Solartron DVM, specify use of . . . . . SHFT-F6 F8, H
Source potentials -- see Ion Optics or Focus
Source-can pressure, query SHFT-F6 F1
Spike, change in middle of manual run SHFT-F8 F9
Spike, define a new SHFT-F7 F3
Spike, delete from disk SHFT-F7 F4
Spike, edit values for SHFT-F7 F6
Spikes, display defined SHFT-F7 F2
Standard-Run Variables, defining/editing/viewing SHFT-F9
Stick, use to change filament-currents from BMS . . . . . Stick U/D
Stick, use to focus ion optics SHFT-F2 F2
Stick, use to rotate barrel SHFT-F3 F1
Stick, use to scan magnet (w. X-Y graphics) SHFT-F1 F4
Stick, use to scan magnet from BMS . . . . . Stick L/R
Stop program (temporarily) . . . . . CTL-Backspace
Strontium model-age, calculate . . . . . CTRL-S
Summary or overview of run-data, display/printout . . . . . SHFT-F8 F3 or F4
Switch magnet DOWN n masses . . . . . CTL-ALT Fn
Switch magnet DOWN to next-defined isotope . . . . . -
Switch magnet UP n masses . . . . . CTL-Fn
Switch magnet UP to next-defined isotope . . . . . +
System-monitor output, graphics monitor of . . . . . SHFT-F6 F9, ALT-G
Temporarily exit auto-running . . . . . F1 →Manual
Time constants of resistor, measure . . . . . CTL-T, SHFT-F6 F10
Time/Date, set . . . . . T, SHFT-F6 F5
Toggle beam-graphics in upper-right of screen . . . . . Esc
Troubleshooting, automatic SHFT-F6 F4
Troubleshooting, general, using graphics-monitor . . . . . SHFT-F6 F9, ALT-G
Troubleshooting, Hall Probe, graphical SHFT-F1 F1
Troubleshooting the focus unit using graphics-scans . . . . . S, SHFT-F2 F3
Tube pressure, query . . . . . CTL-X, SHFT-F6 F1
Tune up beam (center/focus/barrel/center) . . . . . Tab
Turn off filament-current (all filaments) . . . . . 5 (twice)
Turn off filament-current (preheat-center) . . . . . 3 (twice)
Turn off filament-current (preheat-side) . . . . . 4 (twice)
Turn off filament-current (sample-center) . . . . . 1 (twice)
Turn off filament-current (sample-side) . . . . . 2 (twice)
Turret -- see Barrel
User message-file, post message in . . . . . w, SHFT-F5 F7
Vacuum -- see PRESSURE
Version of *Analyst* V
Version of program, printout for QA . . . . . SHFT End

Summary of Functions Available from the *bms*, by MENU

(Note: in the table below, the up-arrow (↑) is used to indicate that the Shift key is to be depressed before the key following; for example, **↑F4 F3** indicates that **Shift F4** is to be pressed, followed by **unshifted F3**)

Unshifted Function-Key Routines: --

Press	To
F1	Center the peak for the current isotope.
F2	Focus the ion optics (automatic).
F3	Optimize the barrel-position.
F4	Change collector from Faraday cup to Daly or vice versa.
F5	Change filament-currents semi-automatically.
F6	Scan magnet semi-automatically.
F7	Change the *Element*.
F8	Rotate the barrel to a new sample.
F9	Take isotope-ratio data in the "manual" mode

Shifted Function-Key Routines: --
(the "shortcut" keys indicate how to access the same function directly from the *bms*)

MAGNET menu (↑F1 from the *bms*) ...

Press	To
F1	Edit the magnet, isotope, or running-data values for an existing *Element*.
F2	Display magnet and running data for the current *Element*.
F3	Do a quick graphics peakshape-check (shortcut: **P**).
F4	Scan the magnet manually, using joystick or cursor-keys, with X-Y graphics (shortcut: **J**)
F5	Adjust magnet-values stored with the *Element* file for magnet or high-voltage drift (shortcut: **M**)
F6	Define a completely new *Element*.
F7	Delete a previously-defined *Element* from disk.
F8	Do a quantitative (slow) peak-flat measurement (shortcut: **~**).
F9	Scan the magnet to determine abundance sensitivity and resolution (shortcut: **Ctrl A**).
F10	Post or remove a flag for one or more *Elements* indicating that the *Element* requires a drift-adjust
↑F1	Do an automatically-scaled magnet-scan with graphics showing the Hall-Probe Output as the Y-axis.
↑F2	Graphically show the variation of magnet-setting with time for the centered position of the most-intense peak of the current or last run (if more than 3 blocks were taken).

FOCUS menu (↑F2 from the *bms*) ...

Press	To
F1	Automatic ion-beam focus (shortcut: **F2** from the *bms*).
F2	Manual ion-beam focus using joystick or cursor-keys (shortcut: **F**).
F3	Scan the focus potentials for any plate, with either beam-size or DAC output as Y-axis (shortcut: **S**).
F4	Display the current focus-settings.
F5	Edit/view/manipulate defined Default-Focus settings.
F7	Query the current accelerating voltage (shortcut: **Ctrl V**).
F8	Type in new focus-settings for any or all plates.
F9	Do a complete beam-tuneup, in the sequence: center peak, focus ion-optics, center peak, optimize barrel, focus ion-optics (shortcut: **Tab**)
F10	Diagnose focus-hardware problems by scanning potentials for all plates and examining ion-beam and DAC response (shortcut: **Alt F**).
↑F1	Change the standard HV setting for one or more *Element*S.
↑F2	Check the stability (drift and noise) of the accelerating voltage.
↑F3	Enable/Disable toggle of before-block printout of accelerating voltage.
↑F4	Show and evaluate the high-voltage drift for the current run or last run (if more than 3 blocks of data taken).

BARREL menu (↑F3 from the *bms*) ...

Press	To
F1	Adjust barrel-position manually. with cursor-keys or joystick.
F2	Test contacts for all samples in barrel and dump graphical record (turns all filaments off) (shortcut: **B**).
F3	Automatic barrel-adjust for largest ion-beam (shortcut: **F3** from *bms*).
F4	Specify safety zones for barrel-centering.
F5	Enter or edit sample names for this barrel (shortcut: **E**).
F6	Display sample names for this barrel (shortcut: **N**).
F7	Replace the exiting barrel-position/Contact-location calibration with the default calibration (use if the last contact-test is suspected to be corrupt).
F8	Store the last calibration of the barrel contact-positions on disk to use as default values.
F9	Display, for the sample currently in running position, the barrel positions where filament-contact is just made and just lost (counterclockwise barrel-rotation), and the amount of backlash in the barrel assembly for this sample.
F10	Inhibit number of barrel-centers allowed during automatic runs.

DALY/CUP menu (↑F4 from the *bms*) ...

Press	To
F1	Toggle between Daly and Faraday Cup detectors (shortcut: **F4** from the *bms*).
F2	Measure the zeroes for both the Daly and Faraday detectors (can do even if a beam is present: shortcut=**Z**).
F3	Calibrate the gain of the Daly detector for the nuclide currently arriving at the collector (shortcut: **Alt D**).
F4	Toggle the Enable/Disable status of the Daly (shortcut: **Ctrl D**).
F5	Temporarily change mass-position of data-taking zeroes for the current *Element* (does not affect *Element* data stored on disk).
F6	Show the zero-drift of the current run for the most-intense peak of that run (if >3 blocks).
F7	Specify the Daly Gain (operator types in a value).
F8	Specify the Daly nonlinearity constant (operator types in a value).

VIEW menu (↑F5 from the *bms*) ...

Press	To
F1	View current *Element* data.
F2	View current Focus settings.
F3	View barrel contact-limits for this sample.
F4	View pressure changes at the start of each block of the current or last run (if >3 blocks).
F5	View changes of magnet-settings, zeroes, and pressure for each block of the current or last run (if >3 blocks).
F6	Browse through the Warning-Message log (shortcut: **Shift W**).
F7	Enter a message in the Warning-Message log (shortcut: **w**).
F8	Shell out (temporary exit) to DOS (shortcut: **Ctrl End**).
F9	Exit *Analyst* and revert to DOS.
F10	Retrieve a screen-image file to screen (shortcut: **Enter**).
↑F1	View sample names for this barrel (shortcut: **N**).
↑F2	View data used to calibrate Source and Flight-Tube pressure queries.
↑F3	Execute a DOS command (shortcut: **Ctrl E**).

HARDWARE menu (↑F6 from the *bms*) ...

Press	To
F1	Query the pressure in the source-can and the flight-tube (shortcut: **Ctrl X**).
F2	Continuous graphical monitoring of the source-can and flight-tube pressures (shortcut: **Ctrl G**).
F3	Query the accelerating voltage (shortcut: **Ctrl V**).
F4	Invoke automatic routines for hardware diagnostics and troubleshooting.
F5	Set the time and date of the computer's clock (shortcut: **T**).
F6	Test the contacts for the filament-assemblies currently in the running and preheat positions (shortcut: **Ctrl F**).
F7	Test the contacts for all of the samples in the barrel (turns filament-currents off: shortcut=**B**).
F8	Edit the hardware-configuration file (shortcut: **H**).
F9	Graphically monitor any computer-interfaced part of the mass spectrometer (shortcut: **Alt G**).
F10	Measure the time constants of the amplifier system (shortcut: **Ctrl T**).
↑F1	Add a point to the pressure-calibration file for either or both of the source-can and flight-tube (shortcut: **%**).
↑F2	Start a new pressure-calibration file for either or both of the source-can and flight-tube.
↑F3	Calibrate either or both of the source-can and flight-tube using the current pressure-calibration file.
↑F4	View the pressure-calibration file.
↑F5	Emulation mode, switch to/from; configure (shortcut: **Alt E**).
↑F6	Initialize the Solartron DVM (if installed).

SPIKES menu (↑F7 from the *bms*) ...

Press	To
F1	See an explanation of *Analyst*'s "Spikes" and how they are used.
F2	Show data for any defined spike.
F3	Define a new normalizable-element spike.
F4	Delete a spike.
F5	Specify a different (or no) spike for the current run.
F6	Edit an existing spike.

DATA menu (↑F8 from the *bms*) ...

Press	To
F1	Take isotope-ratio data in the "manual" mode (shortcut: **F10** from the *bms*).
F2	Enter names for all of the samples in the barrel (shortcut: **E**).
F3	Print or display a Run Summary for one or more runs (shortcut: **Unshifted r**).
F4	Print Run Overviews for one or more *automatic* runs (shortcut: **Shift R**).
F5	Calculate weighted averages of one or more runs (or hand-entered data) (shortcut: **A**).
F6	Locate isotope-ratio data for one or more runs on disk (shortcut: **Ctrl L**).
F7	Transfer current run's data to a tab-delimited DOS RUN*nnn*.DAT file (shortcut: **Alt T**).
F8	Increment the run-number without requiring a sample-change (useful if you're running several different elements from one sample).
F9	Change the sample name for this run.
F10	Change mass-locations of zeroes for this run only (or until next *Element* change).
↑F1	Display the currently-defined sample-names (shortcut: **N**).
↑F2	Specify NdO oxygen & neodymium factors (shortcut: **Ctrl O**).

Non-Function Key Operations (from *bms*)

Keystroke	Action
-	Jump DOWN to next-defined peak
? (or /)	HELP (keystroke index)
+	Jump UP to next-defined peak
*	Enable filament-current change
^	Jump to nearest peak-top
< >	Jump to below (<) or above (>) backgrounds
[ ]	Jump to above or below half-peak position
=	Calculate a radiogenic Pb-207/206 age
%	Add pressure-gauge calibration point
~ (or ')	Quantitative peak-flat measurement
Esc	restore the main BMS screen
Home	Resume auto-running after temporary exit to manual
PageDown	Jump to the ^{187}Re peak (for an Element whose magnet-calibration was defined with a rhenium center-filament current of >4.5 amps)
PageUp	Jump from the ^{187}Re peak to the previous peak
F11	Re-scale beam-chart to include the present beam-size
F12	Toggle beam-noise/beam-growth dials
Enter	Retrieve a screen-file
ALT Enter	Retrieve last-accessed Screen image from disk
CTL Enter	Store present screen on disk
SHFT Home	Re-enter auto running at the start of any run
SHFT End	QA documentation printout (revision date...)
CTL *	(keypad only) Change integration time on beam to 1 second
CTL Backspace	Pause program
CTL Del	Re-start *Analyst* from scratch (power-on state)
CTL End	Shell out to DOS (return with EXIT)
CTL Home	Start auto-running at some arbitrary run
CTL PrintScreen	Print screen-image
Stick button	Enable filament-current change
Stick L/R	Manual magnet-scan from BMS; add SHFT, CTL, or CTL-SHFT to increase speed
Stick U/D	Filament-curr. change using Stick; add SHFT, CTL, or CTL-SHFT to increase response
U/D arrows	Increase, decrease active-filament current
L/R arrows	Change active filament (center-side...) when enabled)
ALT L/R arrow	Scan magnet down/up (slow)
CTL L/R arrow	Scan magnet down/up (fast)
CTL SHFT L/R arrow	Scan magnet down/up (very fast)
1 (twice)	Turn off filament-current (sample-center)
2 (twice)	Turn off filament-current (sample-side)
3 (twice)	Turn off filament-current (preheat-center)
4 (twice)	Turn off filament-current (preheat-side)
5 (twice)	Turn off all filaments)

A ..... Calculate weighted averages of run-data
B ..... Check contacts for all samples in barrel
d (unshifted only) .... Decrease beam-chart "headroom"
D (shifted only) ..... Decrease time shown on beam-chart
E ..... Enter or edit sample-names for a barrel
F ..... Manually focus the ion-beam
G ..... Toggle Log/Linear beam-chart scale
H ..... Edit Hardware Configuration file
J ..... Scan magnet w. joystick or cursor-keys with beamchart
K ..... List functions of common Non-Function-key actions from BMS
L ..... Toggle large/small Beam-chart
M ..... Adjust magnet-values of current Element for drift
N ..... Show names for samples in this barrel
P ..... Quick check of peakshape
Q ..... Blank-out screen with screen-saver (dials only)
r (unshifted only) ..... Print/show data for each block of one or more runs
R (shifted only) ..... Print/show weighted-averages for automatic run(s)
S ..... Scan focus-potentials, graphics display
T ..... Set Time and/or Date
Tab ..... Complete beam-tuneup (center/focus/barrel/focus)
u (unshifted only) .... Increase beam-chart "headroom"
U (shifted only) ..... Increase time shown on beam-chart
V ..... Show version of *Analyst*, operating system, and memory available
w (unshifted only) .... Post message in user message-file
W (shifted only) ..... Look at log of warning or user messages
X ..... Toggle expanded-scale beam-chart
Z ..... Re-take collector zeroes (OK even if a beam is present)

CTL A ..... Scan magnet for abundance-sensitivity and resolution
CTL B ..... Blank-out screen with screen-saver
CTL C ..... Re-check disk for Element data
CTL D ..... Change Daly-Enable status
CTL E ..... Execute a DOS command
CTL F ..... Check filament-contacts (sample and preheat)
CTL G ..... Continuous, graphical monitor of pressure
CTL L ..... Locate run-data on disk
CTL N ..... Calculate a Model-Nd age
CTL O ..... Specify NdO-run oxygen/neodymium correction factors
CTL P ..... Calculate a Pb-isotope Model Age and μ
CTL S ..... Calculate a Model-Sr age
CTL T ..... Calibrate Time-constants of amplifier
CTL V ..... Query accelerating voltage
CTL W ..... Clear warning-message file
CTL X ..... Query pressure

ALT C ..... Quick sample-change (no barrel-reset)
ALT D ..... Calibrate gain of Daly Detector
ALT F ..... Do automatic focus-unit diagnostic-scans
ALT G ..... Invoke graphical output for any device

ALT T . . . . . Transfer current run's data to a (RUN*nnn*.DAT) tab-delimited DOS text file
ALT S . . . . . Initialize the Solartron DVM (if installed)

CTL PrntScrn . . . . . Dump screen to printer
CTL Pause . . . . . Stop (crash) *Analyst* immediately

CTL F(n) . . . . . Jump UP n mass-units
CTL ALT F(n) . . . . . Jump DOWN n mass-units

ALT F2 . . . . . Pause *Analyst*
ALT F3 . . . . . Re-start *Analyst* after a CTL Pause crash
ALT F4 . . . . . Continue *Analyst* after an ALT-F2 pause

Standard Settings of the Mass-Spectrometer for *Analyst*

Analyst requires that the mass-spectrometer switches be set to the following standard settings:

SET	TO
Pirani Ion-Gauge Trip Level	10^{-4}
Electromagnet Supply Programme	Digital
Electromagnet Supply Control	Field
System Monitor	Auto
Digital Integrator Offset	about 5.50 (to get a Cup zero of ~500 cps)
Digital Integrator Response	.03
Digital Integrator Gain	x1
Digital Integrator Timing	1 INT
FA3 Amplifier, Amps-Full-Scale	10^{-5}
" " , Gain	1
" " , Response Time	30 milliseconds
" " , Zero	adjust for a Daly zero of 400-600 cps
Brandenburg, Mains then Reset Button	depress
" , Local/Remote	Local
*Programmable Filament Supply, Centre Fil.	RESET, then ON
* " " " , Man/Auto	Auto
* " " " , EB/TH	TH
* " " " , Side Fils.	RESET, then ON
* " " " , " "	1+2
Programmable Deflection Unit, Mode	Auto
Programmable Focus Unit, Mode	Auto
" " " , Standby/On	ON
Beam Valve (on Flight Tube)	Open
Mains or Power Switches for:	
Pirani Ion-Gauge	ON
Electromagnet Supply	ON
Multiplier Supply	ON
Barrel-Motor Control	ON
Mains Distribution Electronics	ON
Mains Distribution Vacuum	ON
Digital Integrator	ON
FA3 Amplifier	ON
Brandenburg Power Supply	ON
Programmable Focus Unit	ON
Ion-Pump Power Supply	ON

*for both Sample-Filaments and Preheat-Filaments.

ACKNOWLEDGEMENTS

I am indebted to numerous U.S.G.S. and guest researchers for input and patient tolerance of earlier versions of this program and its precursors, particularly Kathleen Simmons, M. Tatsumoto, and John Aleinikoff. Martin Whitehouse provided valuable suggestions on increasing (from nonexistent to almost, but not entirely, nonexistent) the hardware-generality of the program. Wayne Premo and John Aleinikoff provided useful reviews and suggestions for this manual.

REFERENCES

Dodson, M. H., 1978, A linear method for second-degree interpolation in cyclical data collection: Jour. Physics E, v. 11, p. 296.

Hoaglin, D. C., Mosteller, F., and Tukey, J. W., 1983, Understanding Robust and Exploratory Data Analysis. Wiley, New York, N.Y., 447 p.

Ludwig, K. R., 1986, Constraints on time-efficient data-taking strategies for single-collector, isotope-ratio mass-spectrometers: U.S. Geological Survey Bulletin 1622T, p. 219-221.

Russell, W. A., Papanastassiou, D. A., and Tombrello, T. A., 1978, Ca isotope fractionation on the earth and other solar system materials: Geochimica Cosmochimica Acta, v. 42, p. 1075-1090.

INDEX