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User's Guide to DBATIB--A Computer Program for Operation of a Micromass Isomass 54E Mass-Spectrometer

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Manipulating the run-variables

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INTRODUCTION

This program, written for the Isomass 54E instrument installed at the U.S. Geological Survey in Denver, is designed to control almost all instrument operation through the computer keyboard, such that operator attention is minimized in the "manual" (actually semi-automatic) operating mode, and made unnecessary in the automatic operating mode. A major goal of the program is a high degree of flexibility, such that most of the important parameters of data-taking can be customized for different users. As a result, no program alteration should be required to run almost any isotope series manually, or to run most isotope series automatically. The data-taking algorithm is designed to be unusually time-efficient, such that stable runs will yield data with a given accuracy in significantly less time than with most other data-taking algorithms. All data are automatically stored on the DATA tape-cartridge so that statistical and other manipulation of the data can be done without specifically typing in the data. To obtain a listing of the program and/or a copy of the program on tape, write to the author (U.S. Geological Survey, Box 25046, Denver, CO 80225), who will also keep users informed of any crucial revisions.

HARDWARE

The instrument for which DBAT1B was written is an Isomass 54E mass-spectrometer built in 1979 by the Micromass company. This instrument is equipped with a single Faraday cup collector, a 10^{11} ohm resistor, a Daly detector for small ion beams, and a motor-controlled, 16-sample source chamber. The computer is a Hewlett-Packard HP-9835A desk-top computer with I/O ROM and 180 Kbytes of memory, connected to an HP-2631 printer. Because the HP-9835A does not have graphics capability, a strip-chart recorder is used to monitor the ion beam.

GETTING STARTED

You will need 2 operating tape-cartridges for the computer. The first tape (DBAT1B-PROGRAM) contains the running program. The second (DBAT1B-DATA) has the data-files containing running information on the various elements, automatic-running variables and isotope-ratio results. Isotope-ratio data for runs are also stored on this type.

The mass-spectrometer controls must be set to specific standard settings to operate correctly. These setting are as follows:

	Control	Setting
	Pirani ion-gauge trip-level	10^{-4}
	Electromagnet supply programme	digital
	Electromagnet supply control	field
	System monitor	auto
	Digital integrator offset	5.50 (to obtain Faraday Cup zero of about 500/sec.)
	Digital integrator response	.03
	Digital integrator gain	x1
	Digital integrator input	1
1	FA3 amplifier, amps-full-scale	10^{-5}
1	FA3 amplifier gain	1
1	FA3 amplifier response time	30 mS
1	FA3 amplifier zero	adjust to obtain a Daly zero of ~ 500 sec.)
1	Brandenburg, mains, then reset button	pushed
1	Brandenburg, local/remote	local
2	Programmable filament supply, centre filament	reset, then on
2	Programmable filament supply, man/auto	auto
2	Programmable filament supply, EB/TH	TH
2	Programmable filament supply, side filaments	1+2
2	Programmable filament supply, side filaments	reset, then on
	Programmable deflection unit, mode	auto
	Programmable focus unit, mode	auto
	Programmable focus unit, standby/on	on
	Beam-valve	open

1 If Daly is to be enabled.
2 For both sample and preheat filaments.

Mains and power switches to be turned on:

- Pirani ion-gauge
- Electromagnet supply
- [1] Multiplier supply
- Motor control
- Mains distribution electronics
- Distribution electronic
- Mains distribution vacuum
- [1] Digital integrator
- [1] FA3 Amplifier
- Brandenburg power supply
- Programmable focus unit
- Ion pump power supply

The source vacuum should be $<10^{-6}$ torr (preferably $<10^{-7}$), and the tube vacuum (ion pump) $<5 \cdot 10^{-7}$ torr (preferably $<5 \cdot 10^{-8}$).

Put the tape with the running program in the computer and type in GET "DBAT1B", EXECUTE. It takes several minutes to load the program. When the program is loaded (check to see that the yellow light near the tape cartridge stays unlit for at least five seconds), rewind the tape and replace with the "DBAT1B--DATA" tape, then press RUN.

RUNNING THE PROGRAM

First, make sure that you are familiar with the basic operating procedures of the HP-9835A computer, at least as far as knowing how to use the CONTINUE, EXECUTE, and RECALL keys, and how to position the CRT cursor. Also, keep in mind that, once the program is running, pressing the RUN key will re-start the program at the beginning, erase many of the variables, and turn off the filament currents. Thus it is advisable to physically shield the RUN key at this point.

[1] If Daly is to be enabled Brandenberg must also be on.

Starting up

If you have started the program by pressing RUN, you will have to let the computer know a few basic operating parameters. This need be done only once per barrel-load of samples. The procedure is as follows:

CRT Query[1] : [Press continue when printer is ready]

Response[2] : [Indicates that the printer is not on, or not on-line. Press continue when ready.]

CRT Query: ENABLE (1,2) or DISABLE (0) Daly?

Response : Input 0 if you do not wish the Daly detector to be used under any circumstances (for example, if it were non-functional due to hardware failure). Input 1 if you wish the Daly to be used (for small beams) when appropriate or when requested and for data-taking if all peaks are <35 mV. Input 2 if you wish the Daly to be used (for small beams) when appropriate, but not for data-taking. Zero should be input only if the Daly is malfunctioning.

CRT Query : TIME; HOUR, MINUTE, A.M. (0) OR P.M. (1)?

Response : Input 3 numbers indicating the time of day, e.g. 9, 14, 0 for 9:14 A.M.

CRT Query : DATE: MONTH, DAY, YEAR (example: 7,23,82)

Response : Input the date using the indicated format (the example is July 23, 1982).

CRT Query : (1) -Pb; (2) -U/Th; (3) -Sr; (4) -Nd; (5) -HF; ?

Response : The above example is only an example, but shows the format of this query. Input the number corresponding to the element(s) that you wish to run. Data for the(se) element(s) will be loaded from the tape into memory, and the CRT will show which elements and nuclides are in memory, as well as the digital values of the magnet for each nuclide, the normal reference peak, data for normalization (if appropriate) and isobaric-interference corrections, and the HV at which the magnet-values are valid.

[1] In brackets if appearance is conditional.

[2] i.e., type in your response and press CONTINUE.

CRT Query : [7810 VOLTS ADJUST HV TO 7814 (press KO to escape)]

Response : Appears if the high-voltage[1] is different from the required value for the particular element by more than 3 volts (the numbers given above are only examples). The HV will be continually rechecked until you have either (1) changed the HV to the value indicated, or (2) pressed key KO. Normally, the adjustment should be made.

CRT Query : SAMPLE 3, NUMBER OF FILAMENTS?

Response : Input the sample number (defined by the position in the barrel of the sample of interest) of the same that you wish to run, and whether single (1) or triple (2) filament. The appropriate filament assembly will then be rotated into positions (takes 1-3 minutes), and a message such as "SAMPLE #3 IN POSITION 46 108 121" displayed on the CRT. The three numbers indicate the digital barrel positions for the best location of the filament assembly (center number) and the extreme positions where filament contact is still made.

You have now reached the Beam-Monitor Condition.

The Beam-Monitor Condition: (BMC)

At this point, the computer will continuously monitor the intensity of the beam, as well as display which nuclide is being collected, the magnet setting, filament-currents, and which collector is being used. The BMC is thus a "home base" to which the program always returns. Keep in mind that if the computer becomes engaged in a task that you wish ended, or if an error-message appears on the CRT, you can always return to the BMC by pressing STOP twice, then CONTINUE.

A typical display, and its explanation, are given below

Display:

146	Nd	Peak	3917	CF=4.42	SF=1.981	347mV	CUP
a)	b)	c)	d)	e)	e)	f)	g)

[1] The value displayed by the computer, not the setting on the focus-unit.

Explanation:

a) Nuclide that should be arriving at the collector.
b) Dominant element or molecule of this nuclide.
c) Whether on the peak-top ("PEAK"), or off to one side of the peak ("BELOW" or "ABOVE").
d) Fine magnet-setting (proportional to field intensity)
e) Center-filament and side-filament currents, in amperes.
f) Intensity of beam being collected (assumes 10" resistor for Faraday Cup, so 1 mV = 10^{-14} amperes).
g) Faraday Cup ("CUP") or Daly detector ("DALY") as collector.

Note that f) will change up to several times per second.

In this state (BMC) several of the keys on the computer keyboard are activated so that you can instruct the computer to carry out a variety of tasks. It is important to keep in mind that most of these keys "exist" only during the BMC, and also that most of the other (undefined) keys will not function during the BMC. This will be confusing at first, but is a feature that ultimately makes "manual" operation of the mass-spectrometer relatively simple and rapid.

HOW TO OPERATE FROM THE BEAM MONITOR CONDITION [1] [2] [3]

Peak Switching/Scanning

1) Peak-top switching: press the + (plus) key to increment the isotope being monitored. Press the - (minus) key to decrement the isotope.

[1] An overlay card (standard accessory for the HP-9835) for the 12 special function keys should be filled out with mnemonics indicating the function of each key, and placed over the keys.

[2] Note that during the BMC, as well as during most other manual and automatic operations, the computer will reduce the sample-filament current if the peak being collected ever exceeds 10^{-10} ampere (10 volts) and will switch from Daly detector to Faraday cup if the peak being collected exceeds 5×10^{-13} amperes (50 mV). Thus if you wish to hold the filament currents at values yielding beams exceeding these limits, make sure that a minor peak (or no peak at all) is arriving at the collector.

[3] Press (shift) K to obtain a list of defined keys and their functions (Figure 1).

2) Backgrounds: press the ← (left arrow) key to monitor the beam at one-half isotope position below the peaktop, or the → (right arrow) to monitor the background above the peak-top.

3) Peak-sides: press the left parenthesis key to step about one-half of the way down the peak, or the right parenthesis to step about one-half of the way above the peak. These keys are useful for checking centering of the peak.

4) Return to peak-top: press either the ↑ (exponentiation) key or the space-bar.

5) Manual scan: press FORWARD to increase the magnet setting, BACK to decrease.

6) Automatic scan: press (unshifted) K4. The fine magnet-setting for each peak will then appear on the CRT, as will the query, "MIN. MAGNET, MAX. MAGNET, SCAN SPEED (units/sec., to 10,000)?". Choose the range that you wish to scan, and the speed, in magnet units per second. Input these three values (e.g., 3120, 5600, 100). Only up-mass scans are permitted. Make sure the chart recorder is set at a useful speed for the scan. As each peak-top is encountered during the scan, the computer will beep once or twice. If the peaks you wish to scan for are not included in the 0-10,000 range of the fine-magnet settings, answer the first CRT query with all zeroes. The CRT will then query "NEW COARSE MAGNET-RANGE (0-10). The total magnet range, from 0 to 6 amps, is linearly divided into 10 overlapping segments; choose a coarse-range value for input.

7) Peak-shape check: press (unshifted) K3. The magnet will start from just below the top of the peak presently being monitored, scan slowly to just above the peak-top, then reverse direction and scan back to the starting point. Useful chart-recorder speeds for this routine are about 0.5 to 2 mm/second.

8) Switch to ^{187}Re peak: This can be done for element-series that should yield an Re-beam (i.e. high-temperature triple-filament runs). Hold down the CONTROL key and press the - (minus) key.

9) Switch from ^{187}Re peak to regular isotope series: Hold down the CONTROL key, press the + (plus) key.

Changing Detectors

1) Use Daly detector: press (unshifted) K7. If the peak is less than 50 mV, the Daly detector will be switched on, if enabled, after scanning in the region of the peak of interest. If the Daly is disabled, you can enable it (or disable it if enabled) by turning on the FA3 amplifier, multiplier power supply, and Brandenburg, and pressing CONTROL D during the BMC. To calibrate the gain of the Daly detector (which may vary by up to 30%, from week to week),

obtain a peak with between 5 mV and 50 mV intensity, then press (shifted) C during the Beam-Monitor Condition. The calibration subprogram takes about one minute, and is accurate to better than 1% if the beam is stable.

2) Use Faraday Cup Detector: press (unshifted) K6. Note that when switching from the Daly detector to the Faraday Cup, it takes about five seconds before the Faraday Cup will register a beam.

Changing Filament-Currents

1) Manual center-filament change: press (unshifted) + (located at the top center of keyboard) once for each .01 ampere increase, press (unshifted) + once for each .01 ampere decrease.

2) Manual side-filament change: Same as for center-filament, except hold down the shift key while pressing the up-arrow or down-arrow keys.

3) Automatic center-filament change: press (unshifted) K10. The CRT will request two values: the new center-filament current to be reached, and the rate of change of the current, in milliamperes per second. During the process of changing the current, the computer will check the source-pressure every 0.5 amperes, and pause if the pressure exceeds 10^{-6} torr, unless K1 is pressed during filament take-up. If you wish to halt the change of filament-current at any point, press (unshifted) K0. The current change will stop and the computer will revert to the BMC.

4) Automatic side-filament change: Same as above, except press (unshifted) K11 to start.

5) Turn off center-filament: press (shifted) K10. The computer will chirp for 0.5 seconds, during which time you must press (shifted) K10 again. This two-stroke procedure is intended to prevent accidental turn-off of the filaments.

6) Turn off side-filament: Same as above, but press (shifted) K11 twice.

7) Change preheat center-filament: press CONTROL K10. Procedure the same as for sample filaments.

8) Change preheat side-filament: press CONTROL K11. Procedure same as for sample-filaments.

9) Turn off preheat center-filament: press CONTROL SHIFT K10.

10) Turn off preheat side-filament: press CONTROL SHIFT K11.

Automatic Beam Tune-Up Methods

1) Center peak (i.e., find magnet-setting for middle of peak-top): Press (unshifted) K0. If a peak is within 1/2 mass unit or less of being centered, the computer will center on that peak within 1 to 15 seconds. To escape from this routine during execution, press (unshifted) K0.

2) Focus ion optics: Press (unshifted) K1. The computer will automatically adjust all of the focusing potentials for maximum intensity, using no more than four iterations for the seven (eight for triple-filaments) potentials. The time required will range from about 20 seconds to several minutes, depending on how well the beam is already focused, the intensity of the beam, which collector is used, and the stability of the beam (make sure the peak is well centered). You may need to request more than one cycle of four iterations if the beam is very badly out-of-focus. If no beam is apparent, each of the potentials will be scanned over its entire range to search for a beam. To escape from this routine during execution, press (unshifted) K0.

3) Barrel adjust: Press (unshifted) K2. The computer will adjust the barrel for maximum beam intensity. You may need to do this more than once if the barrel was badly out of position. To escape from this routine during execution, press (unshifted) K0. Very rarely, due to a high-voltage arc in the electronics, the barrel will rotate out of control during a barrel-adjust. In most cases when this happens, the computer will turn off the filament currents within a second or two, reset the barrel, rotate the sample back into position, and take the filaments back to running currents. A "RUNAWAY BARREL" message is printed on the CRT and the printer when this procedure occurs.

Note that the accuracy and speed of these beam tune-up routines are dependent on the intensity and stability of the beam. For very low-intensity or very unstable beams, accurate beam tune-up may not be attained.

Manual Beam Tune-Up Methods

1) Manual center: Use the offset switch on the high-voltage panel to switch to the sides of the peak (or use the parenthesis keys on the computer). Adjust the defined peak-top location by scanning with the BACK or FORWARD keys, and when centered press CONTROL * (asterisk) to re-define the peak-top location for the computer.

2) Manual focus: Press (shifted) K3. To increase the potential on a given plate, press the number key for that plate (hold down for steady increase); to decrease, hold down CONTROL while pressing the number key. To escape, press any other key. Ignore beeps arising from the CRT-display overflow. If you are using the Daly, keep in mind that this is one of the few modes wherein the Daly is NOT protected against large beams--so make sure that the beam stays <100 mV.

3) Focus-scan: Press CONTROL K1. You may then scan any focus-control over an arbitrary range and speed to check for malfunctioning hardware. You should put the chart recorder at a suitably rapid speed.

4) Manual barrel adjust: press (shifted K6), then use the up or down arrows at the top center of the keyboard to rotate the barrel up or down. Keep in mind that if you rotate the barrel too far, you will lose contact with the sample and/or preheat filaments. Note that, like the manual-focus routine, the Daly detctor is NOT protected during this procedure.

Sample-Changing/Testing

1) To change sample: Press (unshifted) K8. Enter the new sample number and number of filaments as before.

2) To test contacts of all filament assemblies in a barrel: Press (unshifted) K5. The barrel will rotate through all sample-positions and the CRT will display the apparent number of filaments for each running and preheat sample. A discrepancy between the displayed and actual filament numbers indicates contact problems for that filament-assembly. Note that the Pirani ion-gauge, barrel-motor control, and filament power-supply must be turned on for this test to be valid.

Status Interrogation

1) Read source pressure: press (shifted) K1.

2) Read high voltage: press (shifted) K0.

3) Display time of day and date: press (shifted) T. If the time is obviously inaccurate, an arc probably zeroed the clock. In this case reset with (shift) S.

4) Display fine magnet-settings for isotopes: press (shifted) M.

5) Display focus settings: press (shifted) F.

Miscellaneous Operations

1) To change the isotope-series in memory: press (shifted) K4, and proceed as during start-up of program.

2) To STOP program operation: press STOP or PAUSE.

3) To clear CRT: press (unshifted) CLEAR.

4) To reset clock and calendar: press (shifted) S.

5) To change frequency of beam-monitoring integration: press (unshifted) F ("FAST") to integrate 5 times per second, press (unshifted) S ("SLOW") to integrate once per second. Normally, FAST is more convenient, as SLOW increases the response time to any input.

6) To restore the 'standard' (power-on) focus-values, press control S.

Data-Related Operations:

1) To start a data-taking sequence: press (unshifted) K5 (DATA). For the first block of data only, the CRT will query "SAMPLE NAME?". Enter a name for the sample (up to 50 characters). The CRT will then query either,

a) "ISOTOPES: (REF PEAK FIRST)[; # BLOCKS][, # SETS]?", or,

b) "ISOTOPES: (BESIDES 86 AND 88)[; # BLOCKS][, # SETS]?".

The first query appears if the stored element-series data for the element indicate no internal normalization for mass-fractionation (e.g. Pb, b, Th, single-spiked U), whereas the second query appears if one pair of isotopes is to be used for normalization of mass-fractionation such as for Sr, Nd, Sm, etc. (The actual isotopes given above are only examples). The parameters in brackets are optional (need not be specified), and have default values of 1 block of 10 sets (a set is defined as one peak-switching cycle over all defined isotopes, and a block as a data-taking sequence that includes backgrounds, several sets, and calculations of ratios). Note that a semicolon must be placed before the (optional) # BLOCKS input.

The reference peak is that isotope to which all others are ratioed. Thus if you wished to take data for isotopes 208, 207, and 206, with 206 as the reference peak, your input might be "206, 207, 208" (for 1 block of 10 sets), or "206, 207, 208; 3, 12" (for 3 blocks of 12 sets). Note that except for the first isotope, the order of isotopes is immaterial and does not affect the order in which the peaks are switched. You may take data for up to 6 isotopes and up to 30 sets. There is no limit to the number of blocks (though only data for the last 350 blocks are stored on tape).

In the second case (normalizable element-series), the computer chooses the reference peak and the ratio for normalization, and requests the isotopes

in addition to these two for data-taking. For example, if normalized 87/86 and 84/86 data were desired, the input would be "87, 84" (or "84, 87") for 1 block of 10 sets.

If you wish the filament-current(s) to be turned down (or off) after completion of data-taking for the assigned number of blocks, place an asterisk as the last character of the input. The computer will request the final filament-currents to be reached at the end of the sequence.[1]

If you wish the beam of the most-intense peak restricted within a specified range by adjusting the sample-filament currents, add "$" to the input. The computer will query "MIN. BEAM (mV), MAX. BEAM (mV), MAX SAMPLE-FIL. CURRENT?". Input the desired minimum and maximum beam-size of the most-intense peak, in millivolts, and the maximum sample-filament current, in amperes, that is acceptable. Before each block of data (but not the first block) the sample-filament currents will then be increased (not exceeding the maximum value input) or decreased as required to keep the beam within the specified limits.

If the run is a spiked run of an element with at least 2 constant (nonradiogenic) isotope ratios (e.g. Sr, Nd, Sm), you can request automatic correction for spike isotopes and fractionation (and calculation of sample/spike ratios) by including "*SPK*" in the sample name. The CRT will then query which spike was used (from a list of up to 10 spikes stored on the tape), or request you to define a new spike. This procedure is discussed in more detail in the section on "Data for Spiked Runs".

Before each block of data, all the peaks will be automatically centered, and the peaks quickly monitored to determine 1) the order of peak switching

[1] For Hf-runs only, the ^{187}Re beam will be monitored before each block. If this beam is more than 8 volts, the center-filament current will be reduced.

(always from most intense to least intense), 2) integration time for each peak, 3) delay time (time between start of peak-switch and start of integration), and 4) whether the Faraday cup or Daly detector will be used[1]. In addition, if several blocks of data are requested, the ion beam will be focused before every fourth block.

(More Data-Related Operations):

2) Summary of individual runs[2]: Press (shifted) K9. Remember that runs, samples, and blocks are all different parameters. Input the run-number of interest when requested, and a summary of data for all isotope ratios of all of the blocks of that run will be printed (fig. 5). Press CONTROL K9 for a CRT-printout only.

3) Summary of several runs: Press (shifted) K7. Similar to above, but will print summaries for all runs stored in tape, from 1 to whatever number is specified.

4) Weighted averages of ratios: Press (shifted) K2 to calculate weighed averages of some or all of the isotope ratios of some or all of the blocks for a given run. Refer to the section on this subprogram for more details.

Automatic-Running Keys

1) Press (unshifted) K9 to manipulate run-variables (see separate section in run-variables).

2) Press (shifted) K8 to switch from manual to fully automatic running, or vice-versa (see the section on automatic running for specific information).

DATA-TAKING PROCEDURES

In its simplest form, data-taking proceeds as follows:

1) The source-pressure is monitored; if too high ($>10^{-6}$torr), the computer waits for the pressure to decrease to acceptable limits.

2) (First block of a specified # of blocks only) background (baseline) data are taken. Backgrounds are monitored either at: a) one-half mass position above and below each isotope, or b) one-half mass

[1] The Daly is used only if a) the Daly is enabled with a value of 1, and b) all peaks are less than 35 mV intensity.

[2] A run is defined as the complete sequence of data-taking for a given sample.

position above and below the least-abundant isotope. Type b) backgrounds will be taken only if the Faraday Cup is the collecter, the source-pressure is $<10^{-7}$, and the ratio of most-intense peak to least-intense peak is less than 20. The ratio of peak-top time to background time is chosen to minimize the uncertainty of the ratios for a given total time of data-taking (Ludwig, in press). If a given background position is shared by two peaks, then the background data for this position are shared by the two peaks. The standard deviations of the background readings are calculated, and a 2-sigma rejection applied to the background data. The rejected counts, average counts, and standard deviations are printed out for each background position[1]. If backgrounds above and below a peak differ by a statistically significant amount, a "STEPPED BACKGROUND" message is printed out.

3) Any isobarically interfering elements (defined with ELEMENT data) are monitored unless specifically included in the list of isotopes for data taking.

4) Peak-top data are taken. Delay times (time after peak-switching during which no data is accepted) range from 1 to 4 seconds, depending on the ratio between the previous peak and the present peak.

    a) the average integration time of all the peaks is defined as a function of average peak-intensity, and can range from 4 to 8 seconds per peak,

    b) the integration times for individual peaks are chosen to minimize the uncertainty of the ratios for a perfectly stable beam, (Ludwig, in press),

    c) the integration-times from b) are constrained such that no integration time is less than 2 seconds,

    d) if more than 3 isotopes are involved, the integration time for the least-intense peak is constrained to be equal to the next least-intense peak, and,

    e) if 3 isotopes are involved, the integration time for the least-intense peak is constrained to be no more than 2.3 times that of the second-most intense peak.

    f) if the intensity of any of the monitor isotopes for isobaric interferences indicates a correction of more than 0.05%, the monitor isotope is included in the main peak-top switiching sequence.

[1] For each isotope, the background printout will be (from top to bottom) isotope; below and above-mass backgrounds before peak-top switching; below- and above-mass backgrounds after peak-top switching.

The beam is monitored once per second. Preliminary ratios are displayed for all ratios as each set is completed (normalized for fractionation if required, but not corrected for isobaric interferences). The display line of the CRT (updated every second) displays the isotope that is being collected, its intensity, the set number, and that portion of ion-beam noise in excess of the noise arising from ion-counting statistics and resistor noise.

5) Background data are taken again.

6) Interfering elements for slight (<.05%) corrections are again monitored.

7) Corrections for the resistor time-constants are made by correcting each second's beam-intensity for the propagated resistor decay-effects of all of the preceding seconds' beam intensities. The resistor decay-curve is assumed to be of the form $C_1e^{-T/\tau_1}+C_2e^{-T/\tau_2}+C_3e^{-T/\tau_3}$, as suggested by G. P. Wells of VG Isotopes (oral communication, 1982), where C and τ are constants and T is the time elapsed since a given input to the resistor.

8) Ratios and uncertainties are calculated.

9) If "*SPK*" were included in the sample name, the spike/sample ratio is calculated and, if appropriate, the spike-and fractionation-corrected radiogenic-isotope ratio is calculated.

10) The results for the block are stored on tape.

If the isotopes are 206, 207, 208, 204, and if 206 is the reference peak, then the data taking proceeds in the sequence 206-204; (check peak-top centering); 206-207-208; (check peak-top centering); 206-204. The first and last 206/204 ratios are combined, and 206 background data shared where appropriate. About 40% more total ^{206}Pb-^{204}Pb sets are taken than ^{206}Pb-^{207}Pb-^{208}Pb sets.

DATA PRINTOUT AND CALCULATIONS

Ratios are calculated by linear interpolation using Dodson's algorithm (Dodson, 1978), which corrects for second-order deviations from linearity. These ratios are filtered by a K-sigma rejection routine, where K starts out

at 2 for the first pass, and increases by 0.3 for each successive pass (in order to avoid the over-filtering effect that arises from multiple passes over large numbers of ratios). For elements whose isotope ratios can be corrected for mass-fractionation by normalizing to a standard ratio (e.g. Sr, Nd, Hf, etc.), a linear regression is calculated for the normalizing ratio versus time, and the other ratios are corrected using the regression to estimate fractionation at each time of measurement. The actual fractionation model assumed is the exponential model of Russell and others (1978). Isobaric interference corrections are made assuming a linear growth/decay of the interfering element (for monitor isotopes checked only before and after main peak-switching sequence) or from a least-squares cubic fit with time to the monitor isotope beam (for minor isotopes included in main peak-switching sequence). The results are then printed out for each isotope ratio with the following information (actual numbers and isotopes are examples only).

Explanation of data-block printout (figure 2):

AVERAGE 206/204 -- The mean of the indicated isotope ratios, after rejection for extreme values.

SIGMA % OBS. -- Standard deviation, in percent, of the within-block ratios. Printed in parentheses if a chi-square test shows that this value does not exceed, at the 95%-confidence limit, the standard deviation expected for a perfectly stable beam of the observed intensity (i.e. all of the observed variance is accounted for by ion-counting statistics and resistor-noise.

SIGMA% THEOR. -- The standard deviation, in percent, expected from ion-counting statistics and resistor noise alone (i.e., from a perfectly stable beam; Ludwig, in press).

SIGMA% MEAN -- The standard deviation of the mean of the ratio, in percent. The calculation uses the theoretical sigma if greater than the observed sigma and includes the variance arising from background uncertainty, as well as any variance arising from the uncertainty of the isotope ratio used for mass-fractionation normalization and also

uncertainties in the isobaric interference corrections. Thus the calculated sigma-mean will generally be greater than that calculated by most other programs, reflecting a more rigorous method of calculation rather than a truly poorer precision of measurement.

SIGMA MEAN -- Same as SIGMA% MEAN, but as an absolute value rather than percent.

DELTA % -- The difference, in percent, between the ratio for the present set and the ratio of the previous set. The value is given in parentheses if this difference is not significant at the 95% confidence level.

SETS -- The number of peak-tops used for calculation of the ratios after rejection of extreme values.

mV 208 -- Average intensity of the peak (208 is an example), in millivolts (10^{-14} amperes).

% BEAM-GR./MIN -- The average rate of change of the ion-beam during data-taking, expressed in percent growth of the beam per minute. Thus a decaying beam gives a negative value, a growing beam a positive value.

Other information included in the data printout are the collector-type (Faraday or Daly); the magnet positions for each peak; focus settings; source-pressure at the start of data-taking; sample, block and run numbers; sample name; and time of day and date at the start and end of the run. If interfering isotopes were monitored and their intensities nonzero, the average intensities of the corresponding monitor isotopes are printed out, as well as the average correction from isobaric interferences. If a linear regression of the of the isotope ratios with time shows a change that is significant at the 2.5-sigma level, the magnitude of this ratio-drift is printed out. The amount of correction applied for resistor time-constants ("DZC CORRECTION") is printed out for each ratio. Also, if the ratios were corrected for mass-fractionation by normalizing to a standard ratio (as for Sr, Nd, etc.), the isotopes used for normalization, the apparent degree of mass-fractionation per a.m.u., and the fractionation-uncorrected ratio are printed out.

DATA FOR SPIKED RUNS

If the run is of an element with at least 3 nonradiogenic isotopes of constant ratios (e.g. Sr, Nd, Hf) and you have included the characters "*SPK*" in the sample-name, before taking the first block of data the computer will print out a list of the spikes defined on the tape and request the number of the appropriate spike. If the spike of interest is not stored on the tape, press CONT in response, and the computer will request the appropriate information. This includes the isotope number of 2 nonradiogenic isotopes (in addition to the reference isotope), the isotope number of a radiogenic isotope (if any), and the isotope ratios of the spike and of a standard natural sample.

After each block of data, the computer will define one or two additional ratios besides the actual ratios taken. One of these additional ratios, referred to as "SAM/SPK" is the fractionation- and spike-corrected ratio of the sample reference-isotope to the most-abundant spike-isotope. The other ratio (in the format "87*86"), if a radiogenic isotope is present, is the fractionation and spike-corrected ratio of the radiogenic isotope to reference isotope of the sample. The algorithm used is that of Dodson (1970).

Uncertainties for these ratios include the effects of fractionation and spike-isotope subtraction, but do not include uncertainties in the spike isotope ratios.

NOTE ON USING THE DALY DETECTOR

With the standard settings used for this program, the Daly detector in effect amplifies the ion beam by a factor of 100, with little amplification of noise. This permits more rapid and accurate centering and focusing of small

peaks, so that if the Daly is enabled and the peak is small, the Daly detector is automatically used in beam tune-up routines. The Daly detector can be damaged by exposure to intense ion-beams, however, so that great care has been taken in the program not to permit such an occurrence. Thus under almost all conditions of operation (but not when the program has been stopped for some reason), the intensity of the beam is monitored when the Daly detector is being used. If the beam exceeds 50 mV ($5 \cdot 10^{-13}$ amperes), the Daly detector is turned off and the Faraday cup again used as the collector. This condition obtains during all of the automatic tune-up and data-taking routines, so that the operator should not be concerned if, for example, a beam is being focused an the Daly detector and it is evident that the focusing will yield a much more intense beam. The operator should, however, scrupulously avoid switching to intense peaks with the Daly detector on so that over-intense beam exposures for even a fraction of a second are avoided.

Data-taking using the Daly detector will always yield more precise ratios in less time than the Faraday cup, as ion-counting statistics rather than resistor noise are the dominant source of noise. However, the Daly detector does introduce a bias whose magnitude probably varies from one isotope series to another. Thus unless prepared to do careful calibrations for the isotopes of interest, the operator should accept the fact that data taken with Daly detector have an unknown degree of uncorrected bias (probably in the range of 0.1%-0.6% per a.m.u.).

AUTOMATIC RUNNING

Automatic running implies completely unattended operation of the mass-spectrometer, including sample-changing, filament-current take-up and waiting, and decisions on how much data to take. However, the program is constructed

such that operator intervention during automatic operation is easily done, so that changes of operating specifications, filament-current take-up, beam-tuning, etc., may be done under "manual" (actually semi-automatic) control at arbitrary times during the run if desired.

Run-Variables -- What They Define:

Parameters for automatic running of a given sequence of samples are largely contained in a set of operator-defined variables called run-variables. The run-variables specify the isotopes of interest, the element-series to be run, the order of running of the samples, sample-names, and a set of 27 operating parameters for each run. These operating parameters are stored as array B(i,j) -- j^{th} parameter of i^{th} run (not i^{th} sample)-- and define how sample is to be run. The operating parameters are defined as follows:

Parameter # and Name	Significance
1. SINGLE(1)-TRIPLE(2)	One if a single-filament run, 2 if triple-filament.
2. FOCUSING ISOTOPE	(Only used for triple-filament runs). Defines which isotope (e.g. ^{187}Re, ^{87}Rb) will be used for initial focusing, and for adjusting parameter 3.
3. SINGLE-FIL BEAM (V)	(Only used for triple-filament runs). Defines what beam intensity (in volts) of the isotope of parameter 2 will be required before taking up the side filaments (and thereafter, if this isotope is 187).
4. INITIAL CF (A)	(Only used for triple-filament runs). Defines the initial current, in amperes, that the center filament is to be taken to before adjusting for parameter 3. In other words, this is an estimate of the current required to attain the beam-intensity defined by parameter 3.

5. DALY (0, 1,2)	Zero if the Daly detector is not to be used under any circumstances, 2 if the Daly is to be used (for small beams) when appropriate for beam tune-up routines but not for data-taking, 1 if the Daly can also be used for data-taking (all peaks <35 mV).
6. CURRENT-1	The initial current to which the sample-filament(s) (center for a simple-filament, sides for a triple-filament) are to be taken.
7. RATE-1	The rate, in milliamperes per second, that the sample-filament-current is to change from zero to parameter 6.
8. WAIT-1 (MIN)	The time, in minutes, that the sample-filament current is to be held at parameter 6.
9. CURRENT-2	Similar to parameter 6, except is gained after parameter 8.
10. RATE-2	Similar to parameter 7, but refers to parameter 9. Also used as the rate of sample-filament increase to attain parameter 15 or 18.
11. WAIT-2 (MIN)	Similar to parameter 8, but occurs after parameter 9 is reached.
12. DATA-WAIT (MIN)	Time, in minutes, before data-taking is initiated and after the last change of sample-filament current.
13. ABORT-CURRENT	The sample-filament current, in amperes, above which the run will be aborted.
14. ABORT-WAIT (MIN)	The time, in minutes, that an unstable or steeply declining beam will be tolerated during beam tune-up procedures before either aborting the run or flashing the sample-filament(s).
15. MIN BEAM (V)	The minimum ion-beam intensity, in volts of the most intense peak, that will be permitted before the start of each block of data. If parameter 19 is zero, however, this parameter is ignored after the first block of data. Replaced by parameter 18 once the sample-filament current exceeds parameter 17.

16. MAX BEAM (V)

The maximum ion-beam intensity, in volts of the most intense peak, that will be permitted before reducing the sample-filament current. Applies only to the time just before data-taking for each block, and must be less than 10 volts.

17. DEFAULT CURRENT (A)

The sample-filament current beyond which parameter 15 is replaced by parameter 18.

18. DEFAULT BEAM (V)

The minimum ion-beam intensity (in volts, of the most abundant isotope) that will be accepted once the sample-filament current exceeds parameter 17. Always less than parameter 15.

19. FIL. INCREASE/BLOCK

The amount, in amperes, that the sample-filament current is to be increased after each block of data. Ignored if the ion-beam ever exceeds parameter 16.

20. MIN #BLOCKS

The minimum number of blocks of acceptable data (by the criterion of parameter 22) that will be taken (unless the run is aborted).

21. MAX #BLOCKS

The maximum number of blocks of data that will be taken, regardless of the precision of the ratios.

22. MAX SIGMA (%)

If negative, the negative value of the maximum standard deviation, in percent, of isotope ratios that are permitted for a block of data to count towards parameter 20, whether or not the precision is within theoretical limits. If positive, the precision of all of the isotope ratios of a block must either be less than this value, or be within theoretical limits (of ion-counting statistics plus resistor noise) to count towards parameter 20. All ratios must pass this test to be counted.

23. #SETS/BLOCK

The number of sets taken for each block of data. Must not exceed 30.

24. MAX GROWTH (%/MIN)

The maximum permissible rate of growth, in percent of the ion-beam-intensity per minute. This value applies if one block of data has been taken and if the MIP beam has attained the "MIN BEAM" value. However, if the "DEFAULT BEAM" value has not been reached, no restrictions on growth-rate apply, and for the first block of

	data, or if the MIP beam lies between the "DEFAULT BEAM" and "MIN. BEAM" values, twice the assigned "MAX GROWTH" is permitted. If this value is exceeded, the sample-filament current will be reduced by 2%. This parameter is useful for runs such as single-filament Sr, where growth-rates of more than 2-3% per minute indicate too high a sample-filament current. Can be safely set at 10-15% for insensitive elements such as Pb.
25. PREHEAT CF (A)	The current to which the center filament of the preheat-sample (next-numbered sample) is to be taken and held during the run.
26. PREHEAT SF (A)	Ditto, preheat-sample side-filaments.
27. NORMSPIKE #	If a fractionation-normalized and spiked run, the number of the spike, as stored on tape.

Manipulating the Run-Variables

Run-variables must be defined for all runs before the start of automatic running. This is done by a subprogram that is accessed in the automatic mode as soon as the automatic mode is specified, or from the manual mode by pressing (unshifted) K9. The CRT display will be, "EDIT (1) ADD(2) REPLACE (3) or PRINTOUT (4) RUN-VARIABLES (+ FOR RUN-VARIABLES, - for STD. RUN-VARIABLES CONTINUE to escape)". A sample printout is given in figure 3.

Standard run-variables;

Standard run-variables are a set of up to 32 run-variables for various isotope-series. They can be chosen with a single keystroke, rather than entering all of the run-variables one-by-one for each sample. The standard run-variables are user-defined, and are very convenient if several samples using the same (or even similar) running-pattern are to be run. To see what types of standard runs have been defined in terms of standard run-variables,

input -4 in response to the CRT query above. The type, number, isotopes, and running parameters of all defined standard run-variables stored on the tape will then be printed out (fig. 4).

To replace the standard run-variables stored on the tape, input -3. For each set of standard run-variables, you will then be asked to input:

1) The type of standard run (no more than eight characters long, starting with the element-symbol and the underscore symbol; for example, Pb_XYZ, Sr_4ISO, U_TRIPLE). The element-symbol must correspond to a defined element-series stored on the tape.

2) The isotopes for which ratios are to be taken. These are requested one-by-one. Press CONTINUE when all isotopes (up to 6) have been entered. Note that this does not include monitor-isotopes for isobaric interferences, as these are stored with the element-series information.

3) The 27 operating parameters.

To add more types of standard runs, input -2 in response to the initial CRT query (see first paragraph of this section). Press CONTINUE in response to the "STD RUN # ?" query when all desired additions have been made.

To edit one or more of the 27 operating parameters, input -1 in response to the initial CRT query. The CRT query will then be, "STD RUN #, VARIABLE #, VALUE ?" Input 3 values, separated by commas, defining the number of the standard run-type that you wish to edit, the variable number, and what value you wish that variable to be changed to. When all required changes have been made, press CONTINUE.

The maximum number of standard-variables that can be defined and stored on a given tape is 32.

Run-variables:

Run-variables define how each sample in a given barrel is to be run, and must be re-defined for each barrel-load. Immediately upon selecting AUTO as the running mode, the run-variables subprogram will be accessed, and the "EDIT

(1) ADD (2)...." query will appear. Input 3, indicating that you wish to redefine the run-variables.

The first CRT query for redefining (replacing) the run-variables will be, "SAMPLE # FOR RUN # 1?". Enter the sample number for the first run. The query will repeat, until you have defined the running sequence in terms of sample numbers for the whole barrel (or portion of barrel). Press CONTINUE when the complete running-order (up to 32 runs) has been defined.

The next CRT query will be, "SAMPLE #12 -STANDARD (1) or NEW (2) RUN VARIABLES?" (The sample # is an example). Input 2 if you wish to define a set of run-variables (including operating parameters) that are not represented (or approximated) by the set of standard-variables. The computer will then request the values of the run-variables as described in the section on standard-run-variables. If, however, the isotopes of a standard run-variable type match the isotopes that you wish to take data for, and if most of the running parameters match those that you wish to assign for the run of interest, enter 1. The CRT will then query, "TYPE OF STANDARD RUN (1,2,3,...) for sample # 12?", and will list the types and numbers of standard runs that have been defined. Input the number of the appropriate run-type. The standard run-variables for this run-type will then be assigned as the run-variables for this run. The last CRT query in defining the run-variables for this run will be "SAMPLE NAME FOR SAMPLE #12?" (or other sample #). Input a name (up to 50 characters long) defining the sample.

The above procedure will be repeated until variables for all the samples have been assigned. The complete set of run-variables, as just assigned, will be printed out, and the CRT will display "ENTER 1 TO RETURN TO AUTO CONTROL", or "ENTER 1 TO RETURN TO MANUAL CONTROL" depending on whether you accessed the run-variables subprogram from the automatic or manual mode. If you do not wish to change any of the running parameters, press CONTINUE. Otherwise, input 1 and edit the values as necessary. The computer will then check the accelerating voltage and query if the value is satisfactory. If not, adjust the HV and check again. Remember that all of the runs for this sequence of automatic runs must be at the same HV (within ~3V), and that the computer cannot change the HV. Automatic operation will begin as soon as you accept the HV check.

Note that more than one run may be performed for each sample, and that the filament-current specifications of successive runs for the same sample will start from the existing filament-currents rather than first turning off the filaments. For example, one might wish to take a certain number of 206-207-208 ratios for a radiogenic-Pb run, followed by 206-204 ratios of the same sample but with a more intense ion-beam. In this case, run variables for a 206-207-208 run would be defined, and the subsequent run would be defined as a 206-204 run starting at a higher filament-current. Similarly, one could define a run for $^{238}U/^{235}U$ ratios, followed by a run for $^{232}Th/^{230}Th$ for the same sample, with increased filament-current and decreased beam-intensity requirements.

Running Procedure - Single-Filament Runs[1]

a) (Line Autcont) The sample is rotated into position in front of the source slit, and the filament checked for contact continuity. If an open-circuit is found at this point, and if two more additional attempts at getting filament contact fail, then the run is aborted.

b) Approximate zero (background) readings are taken on the Faraday cup and (if enabled) the Daly detector.

c) (Line Filup) The sample-filament is taken up to the current specified by parameters 6 of the run-variables, at a rate specified by parameter 7. The filament is held at this current for the time of parameter 8. During the period of filament-current increase, the source-pressure is monitored at 0.25 ampere intervals (if >1 ampere) and, if the pressure exceeds $3 \cdot 10^{-7}$ torr, the filament-current increase is stopped until the pressure drops.

d) Same as c), but using the CURRENT-2, RATE-2, and WAIT-2 parameters (parameters 9, 10, and 11).

e) (Line Start) All of the isotopes specified by the run-variables are quickly scanned, and the most intense peak (MIP) identifed. The MIP is centered and the ion-beam focused. If no beam is found, however, the sample-filament current is increased until either a beam appears or the abort-limit is reached (parameter 13). If two successive no-beam aborts occur at this point, automatic operation is suspended (because of the possibility of a persistent hardware fault).

f) The barrel is adjusted for maximum beam-intensity, the beam refocused, the peaks re-scanned, and the MIP re-identified and centered.

g) The MIP is adjusted to be between the limits set by parameters 15 and 16, by changing the sample-filament current.

h) (Line Retake) The beam (of the MIP) is monitored for 10 seconds to check for noise and decay/growth. For the run to proceed, the beam noise must be less than 0.5% per second and rate of change more than -10%. Before the first data-block only, if the beam-growth rate is more than double parameter 24 and the beam more than parameter 15, the sample-filament current(s) will be reduced by 2%. If the noise or beam-decay are not satisfactory within the time of parameter 13, the run will be aborted, (steeply declining beam) or the sample-filaments "flashed" (noisy beam) - i.e., increased by 15%, held there for 2 minutes, then returned to the original current. If the beam remains noisy (after flashing) for the time of the ABORT WAIT parameters, the run is aborted.

i) The MIP is centered, focused, and the barrel adjusted. The beam intensity is checked again for compliance with parameters 15 and 16, and the sample-filament current adjusted as required.

[1] The line identifier in parentheses is the line at which the described procedure is initiated.

j) The preheat-sample filaments are taken to the currents specified by parameters 25 and 26 (before first block of data only).

k) (Line Go) All of the peaks are centered and scanned, and the intensities and ratios of the peaks used for assigning delay and integration times for the subsequent data-taking.

l) (Line Autdat) A block of data is taken, and results for that block printed out. The Beam-growth during the data-block is compared with the MAX. GROWTH parameter, and if it is greater than MAX. GROWTH (MIP greater than the MIN. BEAM parameter) or greater than twice the MAX. GROWTH (MIP less than the MIN. BEAM parameter), the sample-filament current is reduced by 2%.

m) (Line Resume) The results for the block of data are stored on tape. If the block-limits and precision-limits specified by parameters 20, 21, and 22 are met, a summary of the data for all of the blocks taken is printed out (fig. 5), weighted averages for all ratios are printed out (fig. 6), and the next sample is rotated into position. Otherwise, the center-filament current is increased by the current specified by parameter 19, and the running procedure resumes at step (h), with the following differences: the beam is focussed and the barrel adjusted before the first 2 blocks, and for blocks 5, 9, 13.... thereafter.

Running Procedure - Triple-Filament Runs

The procedure is the same as for single-filament runs, except that before step c), the center-filament is taken to the current specified by parameter 4, and the intensity, specified by parameter 3, of the beam of the isotope specified by parameter 2 is reached by further adjustments of the center-filament current. If parameter 3 is zero, however, no intensity-check is performed. This intensity is maintained within 10% of parameter 3 throughout the run.

Intervening During Automatic Operation

Intervention during the automatic operating procedure may be done by stopping the program and pressing CONTINUE to obtain the BMC to request various operations, or by changing the values of the operating parameters while the program in stopped. To resume automatic running where it left off, press (shifted) R during the BMC.

For example, suppose that the automatic running procedure failed to find a beam during the initial beam tune-up, and that the suspected cause was grossly inaccurate magnet positions for the isotopes (perhaps the high voltage had been inadvertantly changed). Press STOP twice, and CONTINUE, and the program would revert to the BMC. Then "manually" find and focus the beam, and then press (shifted) R during the BMC to resume automatic operation.

Or, suppose that, during the seventh run, you changed your mind about the minimum beam intensity that should be allowed during automatic running -- for example, from 1.0 to 1.5 volts. Press STOP twice, type in "B(7,15)=1.5" (see section defining operating parameters), and press EXECUTE. Then press CONTINUE followed by (shifted) R to resume automatic running. Run-variables for samples that are yet to be run can also be changed in this same way.

WEIGHTED AVERAGE AND UNCERTAINTY CALCULATIONS OF POOLED DATA-BLOCKS

Once a run is complete, and the isotope-ratio data for the several blocks of data for that run are stored on tape, a subprogram may be accessed to pool some or all of these blocks for some or all of the isotopes, and to calculate weighted averages and unertainties for the ratios. This subprogram is run automatically at the end of each automatic run, and is manually acessed by pressing (shifted) K2 during the BMC. The CRT will query, "DATA FOR RUN#? (0 to escape, neg. run # if CRT-print only)". Input the number of the run number (not the sample number) whose data you wish to average (input as a positive number if you wish a hard-copy printout, or as a negative number if not). The data for that run will then be loaded into memory from the tape, and the sample-name and isotope ratios for that run will appear on the CRT. The CRT

query will be, "WHICH RATIO (XXX/XXX)?". Input, in the format shown (e.g., 206/207, 87/86 SAM/SPK, etc), the isotope ratio whose data you wish to average. The CRT will then query, "BLOCK #S OF RATIOS NOT TO BE AVERAGED? (press CONTINUE for all)". To reject some of the blocks that contain the isotope ratios of interest, input the block numbers separated by commas (e.g., 3,4,5,9,7). To choose all of the blocks that contain ratios of the isotopes of interest, just press CONTINUE.

The ratios selected will then be weighted according to the inverse square of their standard deviations of the means, and a mean and uncertainty will be calculated. Any ratio whose uncertainty (from both internal and external errors -- see below) cannot account at the 5% confidence limit for the deviation from the mean will be rejected, and a new mean calculated. The probability that the scatter of the individual ratios can be accounted for by their associated uncertainties (internal errors) is also calculated. If no apparent excess scatter exists, the mean and uncertainty are printed out[1]. If, however, significant excess scatter (external error) exists, then this excess scatter is assumed to arise from a constant external source of error (normally distributed). An equation developed by Brent Troutman of the U.S.G.S. (written communication, 1978) is used to estimate the magnitude of this external variance, and this variance is added to the internal (from individual data-block uncertainties) variance to weight the ratios and calculate uncertainties. Because a t-multiplier applies to this external variance component, small numbers of blocks of data with significant external variance will tend to have large uncertainties, compared to the uncertainties of the individual blocks of data, at the 95% confidence level.

[1] For <6 blocks and no apparent external error, the internal errors alone will be used to calculate the uncertainty. For >=6 blocks and no apparent external errors, the actual scatter of the data will be used to calculate the uncertainty.

Definition of terms used in the printout (fig. 6) are:

M.S.W.D.	Mean square of weighted deviates; average value = 1 if internal errors are accurately estimated and if no external errors exist;
Total sigma mean % -	Standard deviation of the mean, calculated from the observed scatter, but with points weighted according to their internal variances.
External sigma -	Calculated external standard deviation required to account for any excess scatter (i.e., scatter not accounted for by internal errors);
Probability -	Probability that the internal errors alone account for the observed scatter; generally in the range of 0.2-0.8 for M.S.W.D. near 1.

DEFINING (OR REDEFINING) DATA FOR DIFFERENT ELEMENTS [1]

Data for running an element-series[2] (I will use strontium as an example) are stored in the tape, and define important parameters for both the instrument hardware and for isotope-ratio data-taking.

TO DEFINE A NEW ELEMENT OR REDEFINE MAGNET-VALUES FOR EXISTING ELEMENT

First, obtain an ion beam of the element of interest, and then press CONTROL T during the BMC. The CRT will query "ENTER 1 IF MAGNET VALUES ONLY

[1] This and the following sections are not of routine interest, and are intended for experienced operator only.

[2] An element-series is defined as a list of nuclides (may include isotopes of more than one element),for which all required magnet-setting information are stored on the tape, plus basic information required for data-taking for one specified element included in the list of isotopes.

ARE TO BE CHANGED, 2 TO CHANGE RUNNING-DATA ONLY, CONT FOR BOTH". If you wish to define a new element (or completely redefine an existing element), press CONTINUE. If you wish to redefine only the magnet and/or HV values for an existing element, enter 1. If you wish to change only non-magnet data (e.g. reference-peak, normalizing ratio, interfering isotopes, etc.), enter 2. If you entered 1 or CONTINUE, the computer will go to the SCAN subroutine. Scan over the magnet-range that you think should include the peaks of interest, changing the coarse magnet-range as necessary. If all peaks are <50 mV, you can scan using the Daly detector. When the last scan includes all the peaks of interest, input 1 to the "OK (1) or RESCAN (2) query. The computer will query the magnet-setting limits over which it is to scan for the peaks for the new element, and then request the element names and integral atomic weights of all of the isotopes of interest by repeatedly querying, "ELEMENT, ISOTOPE #1 (PLUS if >3 mV, MINUS if <=3 mV, CONT when done)" - the isotope # is incremented with each response, of course. A typical input might be "Nd/Ce, 142" for an isotope showing >3 mV peak on the scan, or "Sm, -147" for an isotope showing <3 mV peak on the scan. If the Daly detector was used for the last scan, the peak-height cutoff will be 0.3 mV rather than 3 mV. When all desired isotopes are defined (up to 20), press CONTINUE. The computer will then scan slowly over the specified magnet range, noting each peak as it is encountered. If the number of >3 mV peaks encountered does not match the number that you defined, the computer will abort the procedure and revert to the BMC.

If the number of >3 mV peaks encountered is correct, the computer will scan slowly up and down the sides of the most-intense peak to determine the half-peak offset for isotopes of the new element, and then center each >3 mV peak. The magnet settings of any <=3 mV peaks that were defined will be

calculated by a quadratic interpolation/extrapolation of >3 mV peaks.

Running-data are entered as follows:

CRT Query: TYPE # & NAME?

Response : A number between 1 and 20 to be assigned to this element-series, and a character string defining the main nuclides to be defined (no more than 10 characters). The first character after the element-name must be the underscore character (_). Example: "8,Sr_NORM".

CRT Query: Re-187 COARSE-MAG-RANGE & FINE-MAG SETTING? (CONT IF IRRELEVANT: 8,5770 @ 8 kV)

Response : If ^{187}Re will be present during the runs (as for U, Th, Hf runs), input the correct values - check previously defined element-data if unsure, or scan the spectrum to locate ^{187}Re. If an Re beam won't be present, just press CONTINUE.

CRT Query: REFERENCE ISOTOPE?

Reponse : Input the isotope to which all others are to be ratioed - not a radiogenic isotope if fractionation normalization is possible.

CRT Query: CALCULATED RATIOS AS 86/88 (+1) OR 88/86 (-1)?

Response : The above isotopes are examples. Input 1 if the reference isotope is to appear in the numerator of the ratios, -1 if in the denominator.

CRT QUERY: ISOTOPE FOR FRACTIONATION CORRECTION? (CONT IF NO SUCH ISOTOPE)

Response : If the element has a ratio that does not vary in nature (e.g. Sr, Nd, Hf, Ca), enter the isotope whose ratio with the reference isotope is the standard ratio for fractionation - normalization. If fractionation-normalization is not possible (e.g. Pb, Rb), press CONTINUE.

CRT Query: STANDARD VALUE FOR 86/88?

Response : (The above isotopes are examples). Input the standard value for fractionation-normalization.

CRT Query: HOW MANY ISOBARIC INTERFERENCES?

Response : Input the number of isobarically interfering isotopes that are present (up to 4). Note that more than one element can interfere with one isotope, and that each counts as a separate interference.

CRT Query: MONITOR ISOT., INTERFERING ISOT., INTERF/MONIT RATIO, ALWAYS MONITOR (0,1)?

Response : 4 values. The first value is the number of an isotope that should be monitored before and after the data-taking cycle of peak-top switching. The second value is the isotope of the same element as the monitor isotope, but which isobarically interferes with the element for data-taking. The third value is the abundance of the isotope divided by the abundance of the monitor isotope. The fourth value specifies whether the monitor isotope will be monitored for every block of data-taking (1), or whether it will cease to be monitored after the first block that shows no apparent beam for the monitor isotope. Example: "85,87,.3854,0" for Sr, as the ^{87}Rb interference on ^{87}Sr is corrected for by monitoring ^{85}Rb and corrected using the ratio ^{87}Rb/^{85}Rb = 0.3854 Value 4 is zero because the Rb beam is expected to always be dying under data-taking conditions, and thus the ^{85}Rb beam need only be monitored until it disappears. The above queries will be repeated for each interfering isotope.

The data for the new element-series will then be stored on tape. Up to 20 such element-series may be stored.

APPENDIX I--IMPORTANT PROGRAM VARIABLES

Variable: Bd
Significance: Sample number, according to barrel-location.

Variable: Nm
Significance: Run-number.

Variable: Aut
Significance: Automatic (1) or manual (0) mode.

Variable: F9
Significance: Single (1) or triple (2) filament.

Variable: Ions
Significance: Number of ions per second arriving at the collector for a current of 10^{-14} ampere.

Variable: Daly
Significance: Enabled (1) or disabled (0) Daly detector.

Variable: Mu
Significance: Collector is Faraday cup (0) or Daly detector (1).

Variable: Num (*)
Significance: Number of isotopes whose magnet settings are known.

*Part of element-series variables.

Variable: B1 (*)
Significance: Average difference of fine magnet-settings, per mass-unit, between peaks for the element-series in memory.

Variable: Aside (*)
Significance: Difference between fine magnet-setting at center of peak-top and halfway down the side of that peak, for the element-series in memory.

Variable: N
Significance: Number of isotopes for isotope-ratio data-taking.

Variable: Ref (*)
Significance: Reference isotope for data-taking.

Variable: Rf (*)
Significance: Order of reference isotope in the list of isotopes (Column 2 of array variable A).

Variable: Bar
Significance: Digital barrel-setting for this sample.

Variable: Bara
Significance: Digital Barrel-setting where the filament just loses contact in an upwards rotational direction.

Variable: Barb
Significance: Same as Bara, but in a downwards rotational direction.

Variable: Co(k) (*)
Significance: Coarse magnet-settings for ^{187}Re (k=0) and the other isotopes (k=1) of the list of isotopes (column 2 of array variable A).

Variable: F(k)
Significance: Filament currents. sample-center=F(1), sample-side=F(2), preheat-center=F(3), preheat-side=F(4).

Variable: No(k)
Significance: Noise of mass-spectrometer, in 10^{-14} amperes/second, in no-beam state (dark-noise). k=0 for Faraday cup, k=1 for Daly detector.

Variable: Mx(k)
Significance: Counts per 10^{-14} ampere per second on the digital integrator for Faraday Cup (k=0) and Daly detector (k=1).

Variable: Ze(k)
Significance: Approximate zero-readings, in counts/second, for Faraday (k=0) and Daly (k=1).

*Part of element series variable.

Variable: A(i,j) (*)
Significance: List of isotopes (i) and fine magnet-settings (j) for these isotopes. A(0,2) is the fine magnet-setting for ^{187}Re, A(Rf,2) is the fine magnet-setting for the reference isotope, A(Rf,1) is the nuclide of the reference-isotope.

Variable: A$(i) (*)
Significance: Element (or molecular species) corresponding to the isotopes in A(i,j).

Variable: Mu(i)
Significance: If isotope i (i=order in list of isotopes of A(i,j) is o.k. (known to be <50 mV) for use with the Daly detector, Mu(i)=1. Otherwise, Mu(i) = 0.

Variable: Foc(k)
Significance: The focus settings, where k=1 to 7 corresponds to the plates numbered on the focusing panels, and k=8 reflects the potential between the center and the side filaments.

Variable: Pti(k)
Significance: The integration time, during data-taking, of the k^{th} most intense peak.

Variable: Wt(k)
Significance: The delay time (time before start of integration and after peak-switch) for data-taking of the k^{th} most intense isotope.

Variable: Na$(k)
Significance: The sample name of sample k.

Variable Inv(*)
Significance If ratios are to be calculated with the reference isotope in the numerator, -1 if the denominator.

Variable: B(i,j)
Significance: The j^{th} automatic-running operating parameter for the i^{th} run of a barrel.

Variable: Iso(i,j)
Significance: The j^{th} isotope for data-taking for the i^{th} run.

Variable: Or(k)
Significance: The sample number to be run for the k^{th} run.

Variable: O(k)
Significance: The order, in the list of isotopes (variable A(i,j)), of the k^{th} most intense peak.

Variable: R$(k)
Significance: The isotopes of the ratio of the k^{th} most intense peak, (not counting the reference peak), and the reference peak, in the form "206/207".

Variable: In(k) (*)
Significance: In(1) is the isotope whose ratio with the reference peak is used for normalization of mass-fractionation. In(2) is the isotope ratio of the reference isotope divided by isotope In(1) (i.e., the ratio for normalization).

Variable: If(k,1) (*)
Significance: If(k,1) is the k^{th} isotope used for monitoring for isobaric interference, of the element of interest, by the element of If(k,1). If(k,2) is the corresponding isotope that is an isobaric interference. If(k,3) is 0 if monitoring for If(k,1) is to cease after the If(k,1) beam decays to zero, and is 1 if monitoring is to always occur. If(k,4) is the isotope ratio If(k,2)/If(k,1).

Variable: Av(k)
Significance: The average ratio of the k^{th} isotope-pair of the most recent data-block.

Variable: Acc(k)
Significance: The standard deviation of the mean of Av(k).

Variable: Dzc(k)
Significance: One of the resistor time-constants of the form

$$P = Dzc(1)e^{-T/Dzc(2)} + Dzc(3)e^{-T/Dzc(4)} + Dzc(5)e^{-T/Dzc(6)},$$

where P is the "memory" of the resistor at time T.

Variable: Sig(k)
Significance: The within-run precision of Av(k). Negative if indistinguishable from the theoretical-limiting value.

Variable: Delta(k)
Significance: The difference, in percent, between Av(k) and Av(k) of the previous data-block. Multiplied by $10^{/20}$ if not statistically significant. 10^6 if there are no preceding blocks with this ratio.

Variable: M$(0,1) (= "$OMW0?:0")
Significance: When output to 3, sets detector as Faraday Cup, integration time = 1 second, barrel-motor disabled.

Variable: M$(0,2) (= "$OMW0?60")
Significance: Same as M$(0,1), but with 0.2 second integration-time.

Variable: M$(1,1) (= "$OMW0>:2")
Significance: Same as M$(0,1), but with Daly detector as collector.

Variable: M$(1,2) (="$OMW>62")
Significance: Same as M$(0,2), but with Daly detector as collector.

*Part of element-series variables.

Variable: M$(4,1) (= "$OMWO?:8")
Significance: Same as M$(0,1), but with barrel-motor enabled.

Variable: M$(4,2) (= "$OMWO?68")
Significance: Same as M$(0,2), but with barrel-motor enabled.

Variable: M$(5,1) (= "$OMWO>::")
Significance: Same as M$(1,1) but with barrel-motor enabled.

Variable: M$(5,2) (= "$OMWO>6:")
Significance: Same as M$(1,2), but with barrel-motor enabled.

APPENDIX II - ORGANIZATION OF STORED DATA

The operating tape must contain the following marked data-files:

File TYPE: 20 records of 256 bytes, containing magnet, isotope, nuclide, normalization, and isobaric-interference data for various elements series.

File BEADV: 28 records of 256 bytes, containing run-variables for automatic running (defined by operator for each barrel).

File BSD: 20 records of 256 bytes, containing standard run-variables.

File LRES: 1 record of 10 bytes, containing the file number in RESULT of the last data-block that was stored on this tape. For a newly-created tape, a value of 1 must be printed in this file before first use.

File RESDIR: 32 records of 100 bytes, containing the sample name, sample-number, date, and the file numbers in RESULT of the first and last data-blocks stored.

File RESULT: 350 records of 200 bytes, containing the isotope-ratio means, uncertainties, changes, beam-intensities, isotopes, and block numbers for the last 350 data-blocks.

File SPIKE: 10 records of 150 bytes, containing data for up to 10 spikes

APPENDIX III - TYPICAL PROBLEMS AND SOLUTIONS

Symptom	Possible solution
1. When I press one of the special-function keys, nothing happens.	The SFK's are, in general, operational only during the Beam-Monitor-Condition, and not during most subprogram/subroutines or when the computer is PAUSEd OR STOPped.
2. I answered a query incorrectly and want to STOP this routine and restart it.	Press STOP twice, then CONTINUE. Re-request the subroutine if necessary.
3. The computer indicates that I	If the meters say no current, they're

have current through the filaments, but the current-meters say there isn't.	right. First, turn off the filaments from the computer, then check that all the appropriate filament-supply knobs have been turned to RESET, then to AUTO. Also make sure you've a sample in position.
4. The filaments have been taken to running temperature, but there's no beam.	Check for a beam on the DALY. If present, center and focus. If still no beam, check the filament-currents (the meter not the CRT), make sure that the beam-valve is open, HV is on focus on AUTO, Daly ON if required (Brandenberg meter shows 10-30 kV, FA3 and multiplier power-supply on) and that the magnet meter is in the correct range.
5. The computer doesn't seem to have the ELEMENT data it should.	Either the wrong tape is in the slot or it's not well-seated. Re-RUN the program if necessary.
6. Beam-intensity readings are consistently negative (or consistently too high).	Zeros are wrong. Retake (CTL Z from BMC).
7. When the barrel was rotated to a new sample, the computer beeped and displayed "OPEN CIRCUIT IN SAMPLE" or "USING DEFAULT BARREL-VALUES."	Check that the filament power supply has been RESET and is ON, and on AUTO. Check visually to see if the sample is in position. Check that the barrel-motor switch is ON. Request this "NEW SAMPLE" again. If problem persists, either the filament contacts or the filament itself is probably bad.
8. Isotope ratios are grossly incorrect after correction for isobaric interferences.	Possibly the data for this element has incorrect values. Re-request this element (ELEMENT key from BMC), and carefully check the data that appears on the CRT. OR, the interfering element may not have "natural" isotope ratios.
9. I have to change the HV to get close enough to the peaks for centering.	If consistently off, you may want to re-define the magnet-values for the peaks at a more satisfactory HV. Set the HV to a desirable value (check with the HV key), then press (CONTROL) T from the BMC (see section on defining/redefining elements).
10. The peak shape on the Daly is poor.	Adjust the Brandenburg voltage until peakshape is O.K.

11. The indicated beam-intensity on the Daly is different from that on the Faraday Cup.	Adjust the Multiplier Supply calibration, or request a Daly-Gain calibration (shift C).
12. The program started taking data using the Daly, and the numbers are obviously no good.	The Daly introduces some kind of non-simple discrimination, so that normalizable ratios (Sr, Nd, Hf) are just not valid. Disable the Daly (CTL D, set to 2) otherwise it will be used whenever all the peaks are < 35 mV.
13. The beam keeps completely disappearing, but comes back again in the middle of FOCUS or DATA routines, or after I press PAUSE/STOP, CONTINUE.	Arcs are knocking the focus potentials off. Press STOP twice, then CONTINUE to restore the focus. If the arc frequency is more than about once every 30 min., automatic running may not be reliable.
14. I get data for other runs mixed in with data for the run that I asked to be summarized (or am missing data when retrieved from tape).	Probably either a malfunction during storing the data on tape, or the program was interrupted in the middle of a data-storing operation. Be careful not to interrupt the program while it is storing or retrieving data from tape.
15. The printer stopped printing.	Check that the printer is physically OK (turned on, on-line, etc.). Press STOP twice, then CONTINUE. Press SHIFT R to resume automatic running.

References

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Ludwig, K. R., in press, Constraints on time-efficient data-taking strategies for single-collector, isotope-ratio mass-spectrometer; in U.S. Geol. Survey Professional Paper, Shorter Contributions to Isotope Research.

Russell, W. A., Papanastassiou, D. A., and Tombrello, T. A., 1978, Ca isotope fractionation on the Earth and other solar system materials; Geochim. Cosmochim. Acta, v. 42, p. 1075-1090.

FIGURE 1: PRINTOUT OF KEY-FUNCTION INDEX

KEY	FUNCTION	KEYCODE
K0	CENTER PEAK	-256
K1	FOCUS ION-OPTICS	-255
K2	OPTIMIZE BARREL-POSITION	-254
K3	SCAN FOR PEAK-SHAPE	-253
K4	MAGNET-SCAN	-252
K5	TAKE ISOTOPE-RATIO DATA	-251
K6	USE FARADAY-CUP	-250
K7	USE DALY-DETECTOR	-249
K8	GET NEW SAMPLE	-248
K9	RUN/STD VARIABLES: PRINT,EDIT,REDEFINE	-247
K10	CHANGE SAMPLE CENT. FIL. TO SPECIFIED VALUE	-246
K11	CHANGE SAMPLE SIDE FIL. TO SPECIFIED VALUE	-245
^K0	INTERROGATE HV	-192
^K1	INTERROGATE PRESSURE	-191
^K2	CALCULATE WTD-AVERAGES OF DATA	-190
^K3	MANUAL FOCUS ION-OPTICS	-189
^K4	CHANGE ELEMENTS	-188
^K5	TEST FILAMENT-CONTACTS FOR ALL SAMPLES	-187
^K6	MANUAL BARREL-ADJUST	-186
^K7	PRINT RESULTS FOR SEVERAL RUNS	-185
^K8	START AUTOMATIC-RUNNING	-184
^K9	PRINT RESULTS FOR ONE RUN (PRINTER)	-183
CTL K9	PRINT RESULTS FOR ONE RUN (CRT)	-119
^K10	TURN OFF CENT. FIL. (SAMPLE)	-182
^K11	TURN OFF SIDE FIL. (SAMPLE)	-181
CTL K10	TURN OFF CENT. FIL. (PREHEAT	-54
CTL K11	TURN OFF SIDE-FIL. (PREHEAT)	-53
BACK/FORWARD	STEP MAGNET DOWN/UP ONE UNIT	-206/-208
CTL *	RESET MAGNET-VALUE FOR ISOTOPE	10
SPACE or ^	STEP TO PEAK-TOP	32 or 94
(or)	ABOVE/BELOW PEAK-SIDE	40/41
L/R ARROW	ABOVE/BELOW BASELINE	-234/-233
+ or -	INCREMENT or DECREMENT ISOTOPE	43 or 45
CTL -	STEP TO Re-187 (if defined)	13
CTL +	STEP OFF Re-187	11
STOP/PAUSE	STOP PROGRAM	-204/-239
CLEAR	CLEAR CRT	-203
U/D ARROW	RAISE/LOWER CENT. FIL. (sample)	-232/-231
^ U/D ARROW	RAISE/LOWER SIDE-FIL. (sample)	-168/-167
^F	DISPLAY FOCUS-SETTINGS	102
CTL T	DEFINE NEW ELEMENT-DATA	20
CTL P	RE-STORE ELEMENT-DATA ON TAPE	16
^S	SET CLOCK/CALENDAR	115
^T	INTERROGATE CLOCK/CALENDAR	116
CTL Z	RETAKE COLLECTOR-ZEROES	26
^M	DISPLAY MAGNET-SETTINGS FOR ALL ISOTOPES	109
CTL D	ENABLE or DISABLE DALY	4
F	FAST BEAM-MONITOR (.2 SEC.)	70
S	SLOW BEAM-MONITOR (1 SEC.)	83
REWIND	REWIND TAPE	-211
CTL K1	SCAN FOCUS-VALUES FOR INIVIDUAL PLATES	-127
^R	RESUME AUTOMATIC-RUNNING	110
^C	CALIBRATE DALY-GAIN	99
^K	PRINTOUT INDEX TO BMC-DEFINED KEY-FUNCTIONS	107
CTL S	RESTORE STANDARD FOCUS-VALUES	19

FIGURE 2: SAMPLE PRINTOUT OF DATA-BLOCK

```
XXXXXXXXXXXXXXXXXXXXXXX 5:26 P.M.   NOV 10, 1982 XXXXXXXXXXXXXXXXXXXXXXX
SOURCE PRESSURE = 1.0E-08
SAMPLE#   5                BLOCK#  7                          RUN# 1
CENT. FIL.=2.714 AMPS
PRESSURE =1.0E-08                          20 SETS
SAMPLE: UT-HEN-TM-#1  <.5 u UNSPIKED

                  ISOTOPE     PEAK-T     WAIT-T
                    88           2          1
                    86           5          2
                    87           6          1

FOCUS:   79   0   488   561   269   230   252                    BARREL:   2325
MAGNET: (7737) 88/6719 86/6143 87/6433 85/5853

 88          86          87          85

489/4.2    489/4.2    489/4.2    489/4.2
489/6      489/6      489/6      487/4.8
REJECTED:   469 (85.5)
487/4.5    487/4.5    487/4.5    489/3.8
492/5.1    492/5.1    492/5.1    486/6.7
AVERAGE 85 PEAK =  .0119 mV:    AVERAGE CORRECTION ON 87 = .00103 PERCENT
 634 mV 86
-------------------------------------------------------------------------
********************* 88/86 *********************   FARADAY CUP

 8.40026        8.39959      8.39908      8.39914      8.40052      8.3999
 8.39995        8.40055      8.40037      8.40107      8.40027      8.40046
 8.40147        8.40173      8.39954      8.39984      8.40055      8.40159
 8.40104

RATIO CHANGE DURING BLOCK OF   .0033 % PER MINUTE
DZC CORRECTION  = .00385 %

   AVERAGE        SIGMA%         SIGMA%         SIGMA%         SIGMA
   88/86           OBS.          THEOR.         MEAN           MEAN

   8.40036        (.00919)       .00878         .00249         .000209

   86/88          DELTA%         # SETS         mV 88     % BEAM-GR./MIN
   .119042        .026             20           5320           .39
-------------------------------------------------------------------------
********************* 87/86 *********************   FARADAY CUP

AVERAGE DISCR. CORRECTION =-.152 PERCENT/A.M.U.   (FROM 86/88=.1194)

 .71037        .710455      .710477      .710487      .710376      .71048
 .710438       .710401      .710439      .710474      .710461      .710586
 .710621       .710469      .710357      .710364      .710499      .710403
 .710416
REJECTED:    .710621   .710586

RAW RATIO = .711507
DZC CORRECTION  = .00207 %

   AVERAGE        SIGMA%         SIGMA%         SIGMA%         SIGMA
   87/86           OBS.          THEOR.         MEAN           MEAN

   .710433        (.00664)       .0118          .00326         .0000232

   86/87          DELTA%         # SETS         mV 87     % BEAM-GR./MIN
   1.40759        (.00073)         18             450           .39
-------------------------------------------------------------------------
XXXXXXXXXXXXXXXXXXXXXXX 5:35 P.M.   NOV 10, 1982 XXXXXXXXXXXXXXXXXXXXXXX
```

FIGURE 3: SAMPLE PRINTOUT OF RUN-VARIABLES

RUN-VARIABLES: **********

SAMPLE#	SAMPLE NAME	ISOTOPES				RUN-TYPE
1	SUPRAPUR HCl BLANK, 9/12/82	206	207	208		PB_BLNK
3	HF BLANK, DISTILLED 6/4/80	206	207	208		PB_BLNK
5	NBS STANDARD Pb, SRM-981	206	207	208	204	PB_*4678
2	AR-HA-792A K-FELDSPAR (ACID-WASHED), UNSPIKED	206	207	208	204	PB_*4678
4	AR-HA-792A K-FELDSPAR (ACID-WASHED), SPIKED	206	207	208		PB_678
9	NY-PK-480A/2 ZIRCON	238	235			U_1
7	NY-PK-480A/2 ZIRCON, Pb-UNSPIKED	206	207	208		PB_678
8	NBS STANDARD Sr, SRM-987 (500 nG), #1	84	86	87	88	SR_#2
6	NBS STANDARD Sr, SRM-987 (500 nG), #2	84	86	87	88	SR_#2
10	MI-347A FELDSPAR, Rb-SPIKED	87	85			RB_1
11	MI-349A FELDSPAR, Rb-SPIKED	87	85			RB_1
14	SA-CW-B2 (-200) NM10/20 UNSPIKED	206	207	208	204	PB_*4678
12	SA-CW-B2 (-200) NM10/20 Pb-SPIKED	206	207	208		PB_678
15	UT-HEN-3X-5 (.5 U, UNSPIKED	84	86	87	88	SR_#2
13	UT-HEN-3X-5 (.5 U, SPIKED	84	86	87	88	SR_#2
16	GLASS WAFER #7 (Th)	232	230			TH_

	VARIABLE	SAMPLE NUMBER															
		1	3	5	2	4	9	7	8	6	10	11	14	12	15	13	16
1	SINGLE(1)-TRIPLE(2)	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	FOCUSING ISOTOPE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	SINGLE-FIL BEAM (V)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	INITIAL CF (A)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	DALY (0,1,2)	1	1	0	0	1	1	1	1	1	1	1	0	1	1	1	2
6	CURRENT-1	1.9	1.9	1.8	1.8	1.8	3.5	1.8	2.1	2.1	1.3	1.3	1.8	1.8	2.1	2.1	3.4
7	RATE-1	30	30	10	10	10	20	10	10	10	10	10	10	10	10	10	50
8	WAIT-1 (MIN.)	0	0	1	1	1	2	1	0	0	0	0	1	1	0	0	10
9	CURRENT-2	2.3	2.3	2.2	2.2	2.2	4	2.2	2.5	2.5	1.45	1.45	2.2	2.2	2.5	2.5	4.2
10	RATE-2	10	10	5	5	5	10	5	.15	.15	2	2	5	5	.15	.15	10
11	WAIT-2 (MIN.)	0	0	2	2	2	5	2	10	10	0	0	2	2	10	10	10
12	DATA-WAIT (MIN)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	ABORT-CURRENT	2.7	2.7	2.7	2.7	2.7	4.4	2.7	3.1	3.1	2	2	2.7	2.7	3.1	3.1	4.8
14	ABORT-WAIT (MIN.)	10	10	10	10	10	10	10	10	10	20	20	10	10	10	10	15
15	MIN BEAM (V)	3	3	3	3	3	.5	3	.8	.8	.1	.1	3	3	.8	.8	.3
16	MAX BEAM (V)	7	7	9.9	9.9	9	9	9	7	7	8	8	9.9	9	7	7	2
17	DEFAULT CURRENT	2.45	2.45	2.45	2.45	2.5	4.2	2.5	2.58	2.58	1.6	1.6	2.45	2.5	2.58	2.58	4.5
18	DEFAULT BEAM (V)	.05	.05	.8	.8	.05	.01	.05	.4	.4	.05	.05	.8	.05	.4	.4	.05
19	FIL. INCREASE/BLOCK	.03	.03	.01	.01	.02	.02	.02	0	0	0	0	.01	.02	0	0	0
20	MIN #BLOCKS	2	2	4	4	3	3	3	6	6	3	3	4	3	6	6	5
21	MAX #BLOCKS	4	4	8	8	4	8	4	20	20	8	8	8	4	20	20	10
22	MAX SIGMA(%)	.35	.35	.1	.1	.1	.2	.1	.04	.04	.15	.15	.1	.1	.04	.04	.05
23	#SETS/BLOCK	10	10	10	10	10	10	10	20	20	10	10	10	10	20	20	15
24	MAX. GROWTH (%/MIN.	15	15	15	15	15	15	15	2.2	2.2	3	3	15	15	2.2	2.2	15
25	PREHEAT CF (A)	0	0	0	0	0	3.3	0	0	0	1.3	1.3	0	0	0	0	0
26	PREHEAT SF (A)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	NORMSPIKE#	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	RUN #	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16

FIGURE 4: SAMPLE PRINTOUT OF STANDARD-RUN VARIABLES

STANDARD RUN-VARIABLES **********

STANDARD RUN #	AND TYPE	ISOTOPES
1	PB_6784	206 207 208 204
2	PB_678	206 207 208
3	PB_6/4	206 204
4	PB_BLNK	206 207 208
5	PB_BLNK2	206 207 208 204
6	PB_CONN1	206 207 208 204
7	PB_TRIAL	206 207 208
8	SR_678*1	88 87 86
9	U_1	238 235
10	PB_BLNK3	208 207 206 204
11	SR_SPKD1	84 86 87 88
12	RB_1	87 85
13	TH_1	232 230
14	SR_STD	88 87 86

	VARIABLE	STANDARD-RUN # 1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	SINGLE(1)-TRIPLE(2)	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	FOCUSING ISOTOPE	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	SINGLE-FIL BEAM (V)	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	INITIAL CF (A)	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	DALY (0,1,2)	1	1	1	1	1	0	1	1	1	1	1	1	1	1
6	CURRENT-1	1.8	2	0	2	2	1.8	1.6	2.5	3.5	2	2.5	1.5	4.2	2.3
7	RATE-1	10	20	0	40	200	100	1000	20	20	50	20	10	100	20
8	WAIT-1 (MIN.)	1	1	0	0	0	5	.1	0	2	0	0	0	1	15
9	CURRENT-2	2.2	2.3	2.3	2.4	2.4	2.2	2.2	2.7	4	2.4	2.7	1.7	4.3	2.4
10	RATE-2	5	5	20	10	30	2	500	.15	10	20	.15	2	5	.1
11	WAIT-2 (MIN.)	10	4	0	0	0	15	1	10	5	0	10	10	1	20
12	DATA-WAIT (MIN)	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	ABORT-CURRENT	2.8	2.8	2.8	2.8	2.8	2.65	2.7	3.2	4.4	2.8	3.2	2	4.8	3.2
14	ABORT-WAIT (MIN.)	10	10	10	10	10	10	5	10	10	10	10	10	10	10
15	MIN BEAM (V)	3	3	5	3	1	2	2	2	.5	1	2	1	.005	.35
16	MAX BEAM (V)	9.9	9	8	7	8	9.9	9	6	9	9	6	8	1	6
17	DEFAULT CURRENT	2.5	2.5	2.5	2.45	2.5	2.45	2.4	2.95	4.2	2.5	2.95	1.85	4.5	2.43
18	DEFAULT BEAM (V)	.8	.05	.1	.05	.3	.3	.2	1	.01	.1	1	.01	.001	.15
19	FIL. INCREASE/BLOCK	.01	.02	.03	.03	.03	.01	.02	0	.02	.03	0	0	0	0
20	MIN #BLOCKS	3	3	3	2	1	3	1	8	3	2	6	3	3	8
21	MAX #BLOCKS	6	4	6	4	3	6	1	20	8	4	20	6	6	20
22	MAX SIGMA(%)	.1	.1	.1	.35	.5	.05	1	-.05	.2	1	.04	.15	.3	-.05
23	#SETS/BLOCK	10	12	10	10	10	12	7	20	10	10	20	10	10	20
24	MAX. GROWTH (%/MIN.	15	15	15	15	15	15	15	2.2	15	15	2.2	5	15	2.2
25	PREHEAT CF (A)	1.8	0	0	0	0	2	0	2.4	3.3	0	2.4	1.3	0	2.2
26	PREHEAT SF (A)	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	NORMSPIKE?	0	0	0	0	0	0	0	0	0	0	1	0	0	0

FIGURE 5: SAMPLE PRINTOUT OF DATA-SUMMARY

```
X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*
*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X
```

DATA SUMMARY FOR SAMPLE# 5 RUN# 1 NOV 10, 1982
UT-HEN-TM-#1 (.5 u UNSPIKED

BLOCK#	RATIO	AVERAGE	SIGMA%	SIGMAMEAN%	DELTA%	mV REF. PK
1	88/86	8.37087	.0139	.00349		731
	87/86	.71034	.0205	.00514		
2	88/86	8.38228	.0174	.00432	.14	722
	87/86	.710373	.0149	.00421	(.0047)	
3	88/86	8.38583	.0127	.00304	.042	638
	87/86	.710432	(.00948)	.00326	(.0083)	
4	88/86	8.38978	(.0106)	.00273	.047	664
	87/86	.710411	(.00985)	.00313	(-.0028)	
5	88/86	8.39347	.0172	.0041	.044	695
	87/86	.710373	(.0103)	.0033	(-.0054)	
6	88/86	8.39818	(.00887)	.00233	.056	726
	87/86	.710428	(.00879)	.00293	(.0077)	
7	88/86	8.40036	(.00919)	.00249	.026	634
	87/86	.710433	(.00664)	.00326	(.00073)	
~~8~~	~~88/86~~	~~8.40389~~	~~.0112~~	~~.00293~~	~~.042~~	656
	87/86	.710375	(.0128)	.00354	(-.0082)	

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X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*
*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X*X
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FIGURE 6: SAMPLE PRINTOUT OF WEIGHTED-AVERAGES CALCULATION

BLOCK#	87/86	SIGMAMEAN%
1	.71034	.00514
2	.710373	.00421
3	.710432	.00326
4	.710411	.00313
5	.710373	.0033
6	.710428	.00293
7	.710433	.00326
8	.710375	.00354

WTD AVERAGE 87/86 = .710402 +/- .000022 (.0031 %) (95% CONF. LIMIT)

INTERNAL SIGMAMEAN = .0012 % EST. TOTAL SIGMAMEAN = .0016 %
EXTERNAL SIGMA = .0023 % M.S.W.D. = 1.68 PROBABILITY = .11