PBDAT

A Computer Program for Processing Pb-U-Th Isotope Data

Version 1.24

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TABLE OF CONTENTS

INTRODUCTION

PBDAT takes raw Pb-U-Th isotope data (either typed in from the keyboard or from LOTUS 1-2-3 or other ASCII files), including all relevant data from the chemistry laboratory, and calculates elemental and isotopic concentrations, isotope ratios, apparent ages, uncertainties and error-correlations in these values using the algorithms developed in Ludwig (1980). The resulting data (Table 1) is corrected for instrumental mass-fractionation, laboratory blanks, and the initial Pb of radiogenic samples[2]. Data defining the particular spikes and blanks of a particular laboratory are entered by each user, and stored as user-specific data files on the same disk or directory as *PBDAT* itself. Because of this feature, several different laboratories can use the same program without program modification.

Raw data that has been stored as an ASCII file can be converted by the program as a batch (either in whole or in part) to a reduced-data file which is compatible with the **ISOPLOT** plotting program (Ludwig, 1991). *PBDAT* can accept data from laboratories using a variety of spikes, including ^{208}Pb, ^{206}Pb, ^{205}Pb, ^{235}U, ^{233}U-^{236}U, and ^{230}Th. These spikes can be delivered either to a liquid aliquot or to the total sample, for any combination of Pb and U/Th. Keyboard data-input is managed by a friendly and error-resistant screen which makes extensive use of **HELP** screens and error-trapping.

PBDAT, derived from the **PBDAT200** program for Hewlett-Packard computers (Ludwig, 1985b), is written in QUICK BASIC 4.0 using routines from the PROBAS 3.0 library[3]. If you would like a copy of the current version of this program, write to me directly and enclose a formatted 3½" disk (either 720 Kb or 1.44 Mb) or a formatted, high density (1.2 Mb) 5¼" disk. The source-code, as a text file on another similarly-formatted disk, is also available on request.

The decay constants used by *PBDAT* are those recommended by the I.U.G.S. Subcommission on Geochronology (Steiger and Jäger, 1977): .155125 x 10^{-9} /yr for ^{238}U, .98485 x 10^{-9} /yr for ^{235}U, .049475 x 10^{-9} /yr for ^{232}Th, and present-day $^{238}U/^{235}U$ = 137.88.

HARDWARE REQUIRED

PBDAT requires an IBM-PC compatible computer with at least 384 kbytes of memory, running under DOS 2.0 or later. A Microsoft-compatible mouse is desirable and will be used if installed. The program assumes that the printer is connected to the parallel port (LPT1) of the computer. Use of data files as input (instead of typed-in values) requires a program that can create either space-delimited or tab-delimited text files, such as LOTUS 1-2-3, EXCEL, or even a word-processing program.

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[2]But <u>not</u> for uncertainties in the decay constants of U and Th, nor the uncertainty in the $^{238}U/^{235}U$ ratio of terrestrial uranium. The decay constants and U-isotope ratio used by **PBDAT** are those recommended in Steiger and Jäger (1977).

[3]Hammerly Computer Services, Inc., 9309 Jasmine Court, Laurel MD 20707.

GETTING STARTED

First, look at the READ.ME file that comes with PBDAT for installation instructions and last-minute information. You can do this by typing in **TYPE READ.ME|MORE** and pressing ⤶ . You'll need DOS present either in one of the disk drives (if you're using a two-floppy system) or accessible from the hard disk via the PATH statement in your AUTOEXEC.BAT file. For a hard disk system, copy the *PBDAT* disk onto a subdirectory; for a two-floppy system, put the *PBDAT* disk in the other drive. Change the default drive and path to be that of *PBDAT*, so that the HELP files will be accessible. For example, if *PBDAT* were on the disk in drive **A:** under subdirectory **\PROGS\PB**, you would type **A:** ⤶ , then **CHDIR \PROGS\PB**). Type *PBDAT* ⤶ to start the program. After a few seconds, the screen will display:

```
+)))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))),
*     Files     Input     Output     Spikes     Utilities    LabData     F1=Help     *
*                                                                                     *
*                                                                                     *
*     ##################################################################     *
*     ##                                                                   ##     *
*     ##                                                                   ##     *
*     ##                    6444444444444444447          K.R. Ludwig   ##      *
*     ##                    5                  5            Berkeley    ##     *
*     ## rev. March 18, 1991 5       PBDAT      5          Geochronlogy ##     *
*     ## ver. 1.20          5                  5            Center     ##     *
*     ##                    944444444444444448                        ##      *
*     ##                                                                   ##     *
*     ##         +))))))))))))))))))))))))))))))))))))))))))), ##      *
*     ##         * Spikes:          Pb-208/U-235                    * ##     *
*     ##         *                                                  * ##     *
*     ##         * LabData File:    None                            * ##     *
*     ##         *                                                  * ##     *
*     ##         * Raw-Data File:   None                            * ##     *
*     ##         *                                                  * ##     *
*     ##         * Output to:       Screen Only                     * ##     *
*     ##         .))))))))))))))))))))))))))))))))))))))))))))))- ##      *
*     ##                                                                   ##     *
*     ##################################################################     *
*                                                                                     *
.)))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))))-
```

I'll refer to the above display as the Top-Level Screen.

USING PBDAT'S PULL-DOWN MENUS

Each of the categories listed at the top of the display in the Top-Level Screen has a pull-down menu associated with it. There are several ways of interacting with the pull-down menus:

1)   If you have a mouse, point to the menu-title (at the top of the screen) with the mouse-cursor and click either button. Select an item in the pull-down menu with the mouse by pointing and clicking again, or escape by pointing and clicking outside the menu.

2)   If you don't have a mouse (or don't like to use it), press either the **ALT** key or the slash key (*/*), followed by either (1) the first letter of the menu of interest, or (2) moving the cursor-bar with the left/right arrow-keys to the category of interest and pressing either ⏎ or the up/down arrow-keys.

3)   When you've invoked a pull-down menu, you can select an item without using the mouse by either pressing the key corresponding to the emphasized letter in the item name, or by moving the cursor-bar with the up/down arrows and pressing ⏎ .

Some of the functions in some of the menus are shown in gray characters. These items are inactive, and cannot be selected. If the reason for the status of such an inactive function changes (for example, you cannot reduce data from a datafile until that datafile is loaded into memory), it will become active.

Other functions are either "On" or "Off" -- for example, whether or not the printer is selected for output, or what type of screen is selected. An On/Off function that is "On" will be shown with a check-mark to the left of the function name. Turning an item "On" will cause any incompatible items to be turned "Off" automatically. For example, if you select a Pb-205 spike from the **Spikes** menu, the Pb-208 spike option will automatically be turned "Off".

Some of the functions in the pull-down menus can also be invoked with "shortcut" keys, which will immediately invoke the function without having to invoke a pull-down menu. If such a "shortcut" key exists for a function, it will be shown to the right of the function name in the menu (for example, **F2** to specify printer output). One of the functions in all of the pull-down menus is **HELP**. Selecting **HELP** will give you additional information about the functions in that menu. General **HELP** about the use of the menus and starting *PBDAT* for the first time is available from the top-level menu by pressing either **F1** or **ALT-H**. The first time that you run *PBDAT*, it's a good idea to browse through the pull-down menus and their **HELP** screens.

When you first run *PBDAT*, you'll need to specify what kind of screen you're using before anything else. Invoke the **Output** screen with **ALT-O**, and select either a Color, Monochrome, or "Compaq" screen. The "Compaq" screen option is for monitors that try to emulate a color monitor with different shades of gray (or green, amber, orange...).

Next, specify the format for your reduced-data output and the default location of LabData and raw-data files by selecting the **Output Format & File Location** function from the **Output** menu. The screen should look like this:

```
        CTRL-ENTER=Finished        F9=Recall One        F1=Help


                    Reduced-Data Format and File Location

            Concordia Data: Radiogenic-Pb/2D (1)
                            or Total-Pb/3D (2) ... 1

          Reduced-data format for total-Pb ratios:
                  206/204-207/204-208/204   (1)
              or 204/206-207/206-208/206   (2) ... 1

        Reduced-data format for concordia-plot ratios:
                      206Pb/238U-207Pb/235U   (1),
                      207Pb/206Pb-238U/206Pb   (2),
                  or 206Pb/207Pb-235U/207Pb   (3) ... 1

            Default disk\path for  LabData files ... C:\PBDAT
            Default disk\path for Raw-Data files ... C:\LOTUS

                    Reduced-data file delimited by
                        Spaces (1) or Tabs (2) ... 2
```

Specify whether you want the reduced Pb/U isotopic ratios to be for a 2-dimensional concordia plot (that is, using radiogenic-Pb ratios, with the [207]Pb and [206]Pb corrected for common Pb) or for a 3-dimensional concordia plot ([207]Pb and [206]Pb corrected only for blank Pb).

You can select how you want your reduced-data calculated for both the total-Pb isotope ratios and the radiogenic-Pb isotope ratios. Option 1 for total-Pb ratios will yield data for $^{207}Pb/^{204}Pb$ - $^{206}Pb/^{204}Pb$ isochron plots in which the *slope* of the regression line indicates the age of the system. Option 2 will give you data for $^{207}Pb/^{206}Pb$ - $^{204}Pb/^{206}Pb$ isochron plots, in which the *intercept* indicates the age.

The three concordia-plot ratio options yield formats for U:Pb isotope concordia plots of, respectively, "conventional" style (Wetherill, 1956, Tera-Wasserburg style (Tera and Wasserburg, 1972), and Tatsumoto style (Tatsumoto et al., 1972). Note that the raw-data (input) format is always the same, though.

You can specify the default disk\path for your LabData files and your raw-data files. The first time you run *PBDAT*, these will be the same as the *PBDAT* program. You can change the disk\path for both of these file-types while running *PBDAT*, so don't bother to plan ahead too much at this point.

Reduced-data files can be stored in either a space-delimited format (column-names directly above a row of repeating-equals signs, each column containing 9 characters) or a tab-delimited format (column-names directly above first row of raw data, columns separated by *tab* characters). A tab-delimited format is probably the most generally useful (*ISOPLOT* can read either).

When you're finished, enter the values with **CTRL ↵** and return to the Top Level screen.

<div align="center">

ENTERING DATA FROM THE KEYBOARD

</div>

First, specify a **LabData** file for the program to use (**Load New** from the **LabData** menu). The screen will display a list of the **LabData** files present on the default drive/path. The first time you run the program, just pick any of the example-files shown. More information on **LabData** files is given in a later section.

Using PBDAT's FORM Screens

Start raw-data entry by selecting **From Keyboard** from the **Input** menu (or by simply pressing ↵). The screen will then show:

```
 CTRL-ENTER=Finished    F9=Recall One    F10=Recall All   F1=Help


               SAMPLE, SPIKE, & ALIQUOT WEIGHTS

                             Sample Name ... ??

                  Sample Weight (grams) ... 1
            Total-Aliquot Weight (grams)
             (enter only if appropriate) ... --

           Pb-Unspiked Aliquot (grams) ... 0
             Pb-Spiked Aliquot (grams) ... 1

              U/Th Spiked in Total (1)
         or Pb-Spiked Aliquot  (grams) ... 2

            Pb-Spike delivered (grams) ... 0
             U-Spike delivered (grams) ... 0
            Th Spike delivered (grams) ... 0
```

I call this a FORM screen. When it appears, the response to the **Sample Name** query will be highlighted, indicating where the response-cursor is. Type in a name for the sample whose data you're entering. The double-question marks will disappear, and your sample name will appear in its place as you type it in. Press ⮐ when you've finished typing in the sample name, and the cursor will move down to the next parameter with the sample name remaining where you typed it. To move the response cursor to any parameter, press the up-arrow or down-arrow keys.

To enter a value for a parameter, move the cursor to the appropriate parameter and type in the value. You can edit as you type with the usual cursor-control keys. When you're satisfied with your response, press ⮐ and the value will be entered for that parameter. If you've made an obvious error, *PBDAT* will display an error-message and ask you to re-enter the value. Note that even if you type something into one of the response areas, unless you press ⮐ it will disappear when you move the cursor to another parameter.

When you've entered values for all the required parameters (a double question-mark in a response area indicates that a response for that parameter is required; other parameters may be optional), submit the form by pressing **CTRL ⮐** . Until you do this, none of the values that you entered will be used. If you want to escape from the FORM at any time, press *Esc*. Pressing *Esc* causes the program to ignore all of the values in the FORM that you might have just entered.

If you don't understand the significance of a parameter in the FORM, put the cursor on that parameter and either press **F1** or click on **F1=Help** with the mouse. A **HELP** screen will appear to give you more information on what the significance of that parameter is and what sort of response is required.

If you've already entered a set of values to the form (for a previous sample, for example), you can reuse the last values entered by pressing **F10** (or clicking on **F10=Recall All** with the mouse) when the FORM is displayed. The last-entered values for that FORM will then appear in the current FORM. This feature is especially useful if you made an error in entering the data for a sample but didn't notice the error until after you submitted the FORM, or if you wish to "recycle" data with only slight changes.

The "Weights" Form for ^{208}Pb-Spiked Samples

The above FORM requires values for the various weights involved in a sample analysis. Their significance is as follows:

Sample Weight: -- The weight of the sample that was actually attacked and put into solution, in grams.

Total Aliquot Weight: -- The weight of the total solution of the entire sample, in grams. Enter a value here if you only put a fraction of the total solution of the sample through chemistry; if all of the solution were used (so that the Total Aliquot is just the sum of the Unspiked Aliquot and Spiked Aliquot weights), you needn't enter any value here - *PBDAT* will then assume the Total Aliquot to be the sum of the spiked and unspiked aliquots.

Pb-Unspiked Aliquot (grams): -- The weight of the solution used as the Pb-unspiked aliquot. Samples spiked with Pb before dissolution will have no Pb-unspiked aliquot, nor will blanks. In these cases, enter zero.

Pb-Spiked Aliquot (grams): -- The weight of the solution spiked with ^{208}Pb (or ^{206}Pb).

U/Th-Spiked in Total (1) or Pb-spiked (2) Aliquot: -- If the sample were total-spiked (spiked before attack or before any aliquoting) for U(Th), enter a value of **1**. If the U(Th) spike were added to the same aliquot as the Pb-208 spike, though, enter a value of **2**. Incidentally, *PBDAT* always assumes that if a ^{230}Th spike were used, it was either mixed with the U spike or added to the same aliquot as the U spike.

Pb-Spike (U-Spike, Th-Spike) Delivered (grams): -- The amount of the Pb, U, or Th spikes delivered, in grams. If the Th spike is part of a mixed U-Th spike, then the U and Th spike weights must be the same.

The "Pb-Unspiked Ratios" Form (^{208}Pb-Spiked Samples)

After you submit the completed "WEIGHTS" FORM, the next FORM will be:

```
                  Pb-Unspiked Aliquot Ratios

             (errors must be 2-sigma, in percent)

                        206/204 ... ??
                         %error ... ??

                        206/207 ... ??
                         %error ... ??

                        206/208 ... ??
                         %error ... ??

             Pb-blank (nanograms) ... ??
```

Enter values for the three ratios (raw values from the mass-spectrometer run, NOT corrected for mass fractionation), together with their errors. The errors should be at the 2ó (or 95%-confidence limit) level, in percent, and should correspond to the statistical errors from the mass-spectrometer run, without including the uncertainty due to mass-fractionation.

If you entered a value of zero for the Pb-unspiked aliquot   weight in the previous FORM, the above FORM will ask you for only one ratio: the Pb-unspiked 206/208. Enter your best estimate for the ratio, and

the uncertainty in this estimate. *PBDAT* will then carry these (absolute) values directly through to the reduced-data without corrections for blank-Pb or fractionation.

The **Pb-blank** is the blank that corresponds to the unspiked portion of the analysis only. So if the dissolution process alone contributed a significant amount to the overall blank, you should include only the fraction of the dissolution blank that corresponds to the Pb-unspiked aliquot.

If you didn't measure Pb-isotope ratios for the Pb-unspiked aliquot, just bypass this FORM by pressing *Esc*.

The "Spiked Aliquot" Form (^{208}Pb-Spiked Samples)

The next FORM requires the isotope ratios for the Pb-spiked aliquot, as shown below (assuming a U-235 uranium spike):

```
                       Spiked Aliquot

            (errors must be 2-sigma, in percent)

                          206/207 ... ?
                           %error ... ?

                          206/208 ... ??
                           %error ... ??

                          238/235 ... ??
                           %error ... ??

                          232/230 ... ??
                           %error ... ??

             U Blank (nanograms) ... ??
            Th Blank (nanograms) ... ??
```

The 206/207 ratio for the Pb-spiked aliquot is optional -- if you don't have data for this ratio, don't enter any values for it. *If your sample contains radiogenic Pb, though, you should always include the 206/207 ratio for the Pb-spiked aliquot.* *PBDAT* can then calculate the Pb concentration more accurately, by mathematically compensating for the effect of a varying Pb-blank in the spiked aliquot.

If you didn't enter any Pb-unspiked aliquot ratios, the FORM will also ask for the estimated Pb blank. Enter the Pb blank that corresponds to the Pb-spiked aliquot.

The blank assignments for the U- and Th-ratios should reflect only the blank for the U(Th)-spiked aliquot. You can enter zero if you're sure that the blank is negligible.

The "Initial-Pb Isotope Ratios" Form

If the Pb in the sample is radiogenic and you want to calculate Pb-U-Th isotope apparent ages, you must enter estimated values for the initial-Pb isotope ratios in this FORM. If the Pb in your sample is nonradiogenic (common), or if you're not interested in apparent ages, just escape from this FORM. The initial Pb is defined as the Pb which was present at the time the U-Pb system of interest was "born". For a mineral or rock, this will generally be the Pb present at the time of formation of the mineral or rock.

The FORM for the Initial-Pb ratios is:

```
                    Initial-Pb Isotope Ratios

                 (errors must be 2-sigma, ABSOLUTE)

                       206/206 ... 18.70
                         error ... 0

                       207/204 ... 15.63
                         error ... 0

                       208/204 ... 38.63
                         error ... 0

            206/204 - 207/204
            error-correlation ... 0.9

       F2 Use a Stacey-Kramers Model-Pb for a given age
```

The default values are those for a system with zero age on the Stacey-Kramers Pb-growth curve (Stacey and Kramers, 1975). The errors for the ratios must be entered at the 2ó level and in *absolute* values, not percent values.

Note: Enter nonzero errors for the initial-Pb ratios only if you have reason to believe that the actual initial-Pb isotopic composition was different from sample to sample, or if the sample is not part of a suite. If you're reducing data for several cogenetic samples and you intend to pool the data for a concordia-diagram treatment, enter zero errors even though there is some uncertainty in your estimates of the initial-Pb ratios (you'll have to estimate the effect of the initial-Pb uncertainty by reducing the data-set with different initial ratios, and performing a Yorkfit and concordia-intercept calculation for each set of reduced ratios).

If you do enter nonzero errors for the initial-Pb ratios, you'll need to enter an estimate of the correlation between the 206/204 and 207/204 errors. This value should always be nonzero - typically in the range of 0.8 to 0.95. This error correlation value is the same as the conventional correlation coefficient that you'd get if you do a linear regression of the 207/204 versus 206/204 for several samples that represent the true range of initial-Pb ratios for the system from which your samples were derived. If none of this makes much sense but you still need to enter nonzero errors, an error correlation of 0.9 is probably not too far off.

You can have *PBDAT* use the Stacey-Kramers growth-curve values (Stacey and Kramers, 1975) for any age by pressing **F2** (or clicking on **F2=Stacey Kramers** with the mouse), then entering the Stacey-Kramers age (in Ma). The Pb-isotope ratios defined by the Stacey-Kramers curve for that age will appear in the FORM, after which you can either edit the values, or accept them as given.

Note that much of the information that *PBDAT* can make use of is optional. For example, if you have only the spiked-run data for a 208-spiked Pb aliquot, enter zero for the weight of the Pb-unspiked aliquot. The program will then ask you for only the *estimated* 206/208 of the unspiked run and the uncertainty o that ratio. In such cases, though, you'll need to know all of the Pb ratios (including 206/204) for the spiked aliquot. You needn't enter any U or Th data, nor an estimate for the initial-Pb isotope ratios. When none of the parameters in a FORM are known or relevant, just press ***Esc*** when the FORM appears.

Samples Spiked with a Mixed ^{233}U-^{236}U (-^{230}Th) Spike

For samples spiked with a mixed ^{233}U-^{236}U spike instead of a ^{235}U spike, *PBDAT* accepts two different types of data input. The first type is for data that is already partially reduced so that the Sample-238/Spike-233[1] (SAM/SPK) ratio has already been calculated. This should be the case for data from a mass spectrometer running under ANALYST (Ludwig, 1985a). The Sample-238/Spike-233 ratio is simply the ratio of moles of natural ^{238}U in the U-spiked aliquot to the moles of ^{233}U delivered as the spike. The second type is for raw ^{233}U/^{236}U and ^{233}U/^{238}U ratios. When you specify a U-233/236 spike, *PBDAT* will ask you which type of input to expect.

---

[1]or Sample-238/Spike-236, if U-236 is the most-abundant spike isotope. *This applies to all references to "Sample-238/Spike-236" in this documentation.*

For the first type of data input, the FORM screen will look like this:

```
                    U-Spiked Aliquot

              (errors must be 2-sigma, in percent)


                Sample-238/Spike-233 ... ?
                             %error ... ?

                            232/230 ... ?
                             %error ... ?

                U- Blank (nanograms) ... ?
                Th-Blank (nanograms) ... ?
```

Enter the calculated ratio of the moles of ^{238}U in the U-spiked aliquot of the sample to the moles of ^{233}U that you added from the spike. The rest of the FORM is the same as for ^{235}U-spiked samples.

The second type of 233/236/238 FORM (Sample-238/Spike-233 not calculated) will look like this:

```
                      U-Spiked Aliquot
              (errors must be 2-sigma, in percent)

                       233/236 ...  ?
                        %error ...  ?

                       233/238 ...  ?
                        %error ...  ?

                       232/230 ...  ?
                        %error ...  ?

             U Blank (nanograms) ...  ?
            Th-Blank (nanograms) ...  ?
```

Just enter the raw (uncorrected for fractionation) ratios and errors as usual[1].

_____

[1]If you're using a ^{233}U spike *without* ^{236}U, you can still use this FORM by 1) defining the 233/236 ratio in your LabData file

Samples Spiked with a Mixed ^{205}Pb-U-^{230}Th Spike

For samples that were total-spiked with a mixed ^{205}Pb-U-^{230}Th spike (the U can be either 235 or 233-236), the first FORM will be:

```
            Pb-205 Spiked Sample


                     Sample Name ... ??
            Sample Weight (grams) ... ??
     Pb-205 Spike delivered (grams) ... ??
```

This FORM assumes that the ^{205}Pb spike was delivered to the total sample represented by the sample weight.

The next FORM for a ^{205}Pb-spiked sample is:

```
               Pb-Spiked Aliquot

        (errors must be 2-sigma, in percent)

                     206/204 ... ??
                      %error ... ??

                     206/207 ... ??
                      %error ... ??

                     206/208 ... ??
                      %error ... ??

                     206/205 ... ??
                      %error ... ??

         Pb-Blank (nanograms) ... ??
```

---

to be 1.000, then 2) entering a value of 1 + 3F/100 for the 233/236 ratio in the FORM, where F is the predicted mass-fractionation for your uranium runs, in percent per mass-unit.

The Pb blank is the blank that corresponds to the complete attack, extraction (if any), and loading procedure. The rest of the data input (for ^{205}Pb-U-Th spiked samples) is the same as for ^{208}Pb-spiked samples.

Entering Data for Blank Determinations

For Pb-blanks, you usually won't have any specific data for the Pb-unspiked aliquot ratios, and you might not have any data for the Pb-spiked 206/204 ratio. So for blanks, enter the weight of the Pb-unspiked aliquot as zero (since there wasn't any unspiked aliquot). *PBDAT* will still ask you for an estimated value for the unspiked 206/208 ratio, however. Enter your best guess for this value (unless your blank is very underspiked, your guess doesn't have to be too accurate). You'll also need to enter an uncertainty in your estimate -- 5% isn't too large if you know only that the blank Pb is a "normal" common Pb (206/208 = 0.46-0.50).

The Pb-Blank value that you enter into the Pb-Spiked Aliquot Ratios FORM will depend on what type of blank-determination you're doing. For a total-blank, enter a blank-value of zero (you want to know the total contamination). For a reagent blank, though, you should enter the estimated blank for loading plus whatever handling (evaporation, weighing...) accompanied the blank procedure. It's worth noting that for blanks of very pure reagents (for example, water), the evaporation blank can easily exceed the reagent blank itself.

Entering Data for Spike-Concentration Calibrations

Isotope Ratios of Spike Known: To calibrate the concentrations of a spike, you'll need to have (1) a standard solution or solid with known isotope ratios and concentrations, (2) an isotopic analysis of a (well mixed) mixture of the standard and the spike, and (3) an estimate of the true (blank-corrected) ratios of the spike. Enter the data into *PBDAT* in the following way:

Sample weight:	Weight of the standard solution (or solid).
Total-aliquot weight:	Zero
Pb-Unspiked Aliquot weight:	Zero
Pb-Spiked Aliquot weight:	1
U/Th-spiked in total (1) or Pb-spiked (2) aliquot:	1
Pb, U, or Th Spike, grams delivered:	Weight of the spike delivered to the mixture.
Blank amounts:	The nanograms of Pb, U, or Th contamination that you assign to the mixing, loading, running, and (if a solid standard) dissolution procedure. But enter *zero* for the Pb-unspiked aliquot blank
Pb-isotope ratios:	For the unspiked aliquot, enter just the (accepted or known) 206/208 ratio for the *standard*. For the spiked aliquot, enter the observed ratios of the mixture.

Unless you have a combined Pb-U-Th standard, you can only reduce the data for one elemental-spike at a time, even though all three elements were combined in the mixing stage.

Examine the indicated concentration of the major spike-isotope in the *PBDAT* printout. This is the indicated concentration of that isotope in your standard using the presently-defined concentration of your spike. The percent difference in the concentration that you just obtained for the standard is the amount that you need to adjust your spike concentration; to make this adjustment, change the spike concentration in the **LabData** file by the percent difference above, but in the *opposite* direction.

In other words, if the spike-calibration run indicates that your standard is 1% too *high* compared to its accepted value, then *lower* the spike concentration in the **LabData** file by 1%. If the indicated standard concentration were 1% too *low*, then *increase* the spike concentration in the **LabData** file.

Isotope Ratios of Spike Unknown: If you don't have any reliable data for the isotope ratios of a new Pb-208 (or 206 or 207 or 204) spike, though, you can do the following procedure to get both the spike's concentration and blank-corrected ratios. Do 2 isotopic analyses of the new spike: one as just the pure spike, in a relatively large amount (to swamp out any loading/handling blank); the other as a mix with your

usual standard. Now define a **LabData** file whose Pb-208 spike is the *standard* used in the mixed analysis. This standard could be a calibrated common-Pb solution, a pure Pb-206 solution, or a solid standard.

Reduce the data, using the **LabData** file as defined above, as follows:

Sample weight:	Sum of the weights of a) the new spike used for the first (pure spike) analysis, and b) for the second (mixed) analysis.
Total-aliquot weight:	ignore
Pb-Unspiked Aliquot weight:	Weight of the new spike used in the first (pure) analysis.
Pb-Spiked Aliquot weight:	Weight of the new spike used in the second (mixed) analysis.
U/Th-spiked in total (1) or Pb-spiked (2) aliquot:	2
Pb, U, or Th Spike, grams delivered:	Weight of the *standard* delivered to the second (mixed) analysis.
Blank amounts:	Nanograms of Pb blank that pertains to the delivery, evaporation, and loading of the new spike for the first (pure spike) analysis.
Pb-isotope ratios:	For the unspiked aliquot, enter the ratios from the first (pure spike) analysis. For the spiked aliquot, enter the ratios from the second (mixed) analysis.

CREATING AND USING RAW-DATA FILES

The best method for reducing data for more than one or two samples at a time is to put the raw data in a text file, so that you can edit the raw data at any time or re-reduce some of the data with new **LabData** file values without having to re-enter a lot of data. You can create these files with LOTUS 1-2-3[1], EXCEL, most other spreadsheet programs, or with any word processing program that can create ASCII files.

PBDAT can read two types of text files: space-delimited and tab-delimited.

---

[1]Use the **/PF** command (PRINT FILE), which will create a space-delimited, ***.PRN** file.

Space-Delimited Raw-Data Files

Space-delimited files can be created by LOTUS 1-2-3, and by most word-processing programs. The numeric data-columns must all be 9 characters wide, and the sample-names must be in the left-most column (18 characters wide) or 2 columns (each 9 characters wide). Store the raw data as an ASCII file with a left margin of 0 and a right margin large enough to include all of the relevant columns (= # of columns times 9). You can use the Lotus TEMPLATE file (on the PBDAT program disk) as a guide. This file will give you the correct format and column-headings for your raw-data files (the different rows of the TEMPLATE file are for different ways of spiking: excise the appropriate one). If you store the raw-data file from LOTUS (using the PRINT FILE or ASCII FILE option), make sure that the range you specify includes all of the required parts of the spreadsheet. Include all 9 characters of the right-most column. The numeric data in the file must be separated from any titles or column-headers by a line of repeating-equals signs whose length is equal to the number of raw-data columns times 9.

Tab-Delimited Raw-Data Files

Tab-delimited files are the text files created by some spreadsheet programs (such as EXCEL) and by most Macintosh programs. Put the sample names in the left-most column (only the first 18 characters will be used by PBDAT). PBDAT will take as the first row of raw data the first row in the file that contains either an asterisk in the sample-name column (indicating the presence of an embedded specifier), or any other characters in the sample-name column PLUS a numeric value in the first numeric raw-data column (=the sample-weight column).

Both Types of Raw-Data Files

The file must be arranged in rows and columns like a spreadsheet, with different samples occupying different rows. The top row of the raw-data spreadsheet can be used for a title of up to 80 characters, and will appear on the screen when you access the file from PBDAT. You can look at the contents of the currently-selected file by pressing the **FILE PREVIEW** (**F3**) from the "Load File" screen. When the file appears on the screen, use the cursor keys to move the screen "window" to any part of the file.

If you don't have any data for one of the columns, or if that column is irrelevant (for example, thorium data when you didn't spike the sample for thorium), don't enter anything in that column. Enter all errors (uncertainties) at the 2ó level and in percent.

Note that the columns for uranium isotope ratios can contain either the 238/235 ratio, the Sample-238/Spike-233 ratio, or the 233/238 ratio. The program will assume one of these, depending on (1) whether the sample were spiked with a Pb-205 mixed spike, in which case the **LabData** file will specify a 235 or 233/236 U-spike, (2) whether you specified a U-235 or U-233/236 spike from the Top-Level CRT display, (3) which data-input format for U-233/U-236 spiked samples you are using, and (4) if you have embedded specifiers (see below) within the sample name columns of the raw-data spreadsheet.

If your data is for ^{233}U-^{236}U spiked samples with raw 233/236 and 233/238 ratios, the 233/236 ratios and errors must occupy the last two columns of the spreadsheet (AB and AC for 208-spiked samples, T and U for Pb-205 spiked samples).

Using Embedded Specifiers within the Raw-Data File

The raw-data spreadsheet can contain all of the necessary information to tell the program how the data is to be reduced, including which **LabData** file to use, whether spiked with Pb-208 or Pb-205, U-235 or U-233/236, whether the U-Th was spiked in the total aliquot or the Pb-spiked aliquot, and what initial-Pb ratios to use. These specifiers can change from sample to sample, so that a large raw-data spreadsheet can contain data reduced at various times (or by various laboratories), with different spikes and procedures, yet the whole file can be reduced in a single request that creates a single reduced-data file.

Embedded specifiers consist of a few characters enclosed in asterisks, and must occur within the sample name column(s). The specifiers affect how data for samples below the specifiers are reduced. The types of embedded specifiers that you can use are shown below:

SPECIFIER SIGNIFICANCE

L   The characters following the specifier indicate the name of the **LabData** file to be used (for example, ***L* C:\PBDAT\NEWLAB**)[1].

205   Samples were spiked with a mixed 205Pb/U/Th spike (the **LabData** file for the spike determines whether a ^{235}U or ^{233}U-^{236}U spike is assumed.

208   Samples were spiked with a ^{208}Pb or ^{206}Pb spike.

235   Samples were spiked with a ^{235}U spike (208-spiked samples only).

233   Samples were spiked with a mixed ^{233}U-^{236}U-spike (208-spiked samples only).

TU   Samples were total-spiked with U(Th).

PU   Samples were spiked for U(Th) in the Pb-spiked aliquot.

---

[1]If the full path and LabData file name are too long to fit in the 18 characters allotted for the sample name, you'll have to type in just the *name* of the LabData file and either (a) enter the disk\path for the LabData file at the time of data reduction when PBDAT asks you (after failing to find the file on the default LabData path), or (b) change the default LabData path to match the LabData file.

SAMSPK Raw data for any ^{233}U-^{236}U spiked samples will be in the form of Sample-238/Spike-233 ratios rather than the raw 233/236 and 233/238 ratios.

368 Raw data for any ^{233}U-^{236}U spiked samples will be in the form of raw 233/236 and 233/238 ratios.

INIT Use the values in this row as the initial-Pb ratios and uncertainties. From columns C to I, respectively, the cells in this row will contain values for the initial-Pb 206/204, 6/4-error, 207/204, 7/4-error, 208/204, 8/4-error, and 206/204-207/204 error-correlation. See below, however, for obtaining Pb ratios for a Stacey-Kramers Pb-evolution in a simpler way.

SK Use the number following this specifier to calculate a Stacey-Kramers single-stage Pb[1] to use for the initial-Pb ratios (for example, ***SK* 1750**). The uncertainty in these ratios will be set to zero.

Note that if you want to reduce just part of the data in a raw-data file, you must include the row numbers of the appropriate embedded specifiers in the sample numbers that you request. Otherwise, PBDAT will never access the embedded specifiers to be able to do what you want. So if the embedded specifiers of interest occur in, say, row 13 of the raw-data spreadsheet followed by the actual data in rows 14 through 20, you would have to include the "sample number" for row 13 for the embedded specifiers to work (see example below). You'll be able to tell which "sample number" to use from the printout or display when you access the raw-data file from PBDAT.

Accessing Raw-Data Files

To load a raw-data file into memory, select **Load Raw-Data File** from the **Files** menu. The screen will display all files in the current disk and directory (the default path for raw-data files is shown in PBDAT's **CONFIGURE** screen), as well as any other paths accessible from the current path. Select a file or a path by moving the file-cursor with the cursor-control keys or with the key for the first letter of the file or path name (for example, press **H** to jump to the first file starting with the letter H, press **H** again to jump to the second file starting with H, and so on).

Path names are indicated with a backslash at the end, and the parent directory (which is always present) is shown by the usual DOS label of **..**. Change the disk or path to search with the **F2** key if the file or path that you want isn't shown.

The default file-extension for raw-data files is **.RAW** (**.RED** or **TXT** for reduced-data files). Only files with this extension will appear in the directory screen. You can change the extension that raw-data files

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[1]Stacey and Kramers, 1975.

must have with the **F8** key (**Change Extension**) - but note that except for a specified extension of **.*** (all files shown), the DOS wildcard characters (***** and **?**) will not function.

Once you've selected a file, the screen will show the file's title and sample names as they are accessed from the disk, as well as a few of the isotope ratios for the samples. A typical display might look like this:

```
East Dakota Zircons, 1440 Ma initial

#       NAME               Wt (g)   206/204    206/207    206/208
1: *L* C:\PB\OLDLAB         ---       ---        ---        ---
2: *208* *TU*               ---       ---        ---        ---
3: *INIT*                  16.162     ---        ---        ---
4: 84/TL 1043 -200         .05432   1012.2     10.113     14.125
5: 84/TL 1043 -100+150     .03156   734.24      8.2361    10.113
6: 84/TL K-feldspar        .1043    16.129      1.0458     .465211
7: *PU*
8: 88/ZE 53A -400 1.7nm .0835      15421       15.663     18.943
```

The top line of the screen shows the title of the raw-data file that you put in the top row of the raw-data spreadsheet. Note the embedded specifiers.

Reducing Data from a Raw-Data File

Once a raw-data file is in memory, *PBDAT* will display the screen below, you can reduce it either by selecting **From Datafile** from the **Input** menu, or by simply pressing **CTRL ⏎** . *PBDAT* will then ask you to:

```
 F2=All Sets                                         F1=Help


                                     +)))))))))))))))))),
     ENTER SAMPLE NUMBERS TO BE REDUCED: *1,32             *
                                     .))))))))))))))))))-


 Separate the sample-numbers of a continuous sequence with a
 comma, and separate different sequences of individual samples
 with a semicolon (example: 1,5;12,15;21).  Be sure to include
 rows with embedded specifiers.
```

Separate the sample-numbers of a continuous sequence with a comma, and separate different sequences or individual samples with a semicolon (example: 1,5;12,15;21). Be sure to include rows with embedded specifiers.

The output of the reduced data depends on the selections from the **Output** menu. If **Pause Screen for Viewing** is selected , the screen output will pause with each full screen until a key is pressed; if "Off", the screen will scroll continuously as the results are calculated.   If **43-line Screen** is selected (requires an EGA or VGA monitor), the screen will contain 43 lines when full, instead of 25 lines. If **Suppress Screen** is selected, only the sample names will be shown on the screen as the data is reduced (automatic for printer output; also useful for datafile data-reduction where the results will be stored in a reduced-data file). If **Printer** is selected, all of the output will be directed to the printer instead of the screen.

You can now reduce the data in the raw-data file. If you want to reduce data for all of the samples in the raw-data file, just press the **ALL** key (**F2**). If you want to reduce only part of the data, indicate the sample-numbers of continuous sequences of data by entering the first and last number of the sequence separated by a comma, and indicate discrete sample-numbers or the start of a different continuous sequence by a semicolon. So to specify that sample numbers 1 though 6, then 9, then 12 through 15 be reduced, you would enter **1,6;9;12,15**.

Remember to include rows containing any embedded specifiers if you want those embedded specifiers to take effect. Remember also that once an embedded specifier is acted upon, it remains in effect until specifically canceled by either another embedded specifier or by softkey-commands from the Top-Level Screen.

After you've specified which samples in the datafile to reduce, the program will display the Initial-Pb Ratios FORM. Enter the initial-Pb ratios as discussed earlier (or press *Esc* if you don't want apparent ages to be calculated for any of the samples, or if the initial-Pb ratios are specified in the raw-data file itself). The data will then be reduced.

CREATING AND USING REDUCED-DATA FILES

After all the samples in the raw-data file have been reduced (unless you've only reduced data for one or two samples), the screen will ask you to specify a name for a reduced-data file. The screen will show you the default path and extension (**.RED**). If you want a different disk\path or extension, enter the desired disk\path\filename. You can specify a tab- or space-delimited file format with the **F2** key.

PBDAT will now ask you for the format of the reduced-data file: "Zircon", "Whole-Rock", or "Complete." If you store all of the reduced-data ratios and errors that PBDAT calculates ("Complete" format -- see Table 3) you won't be able to access the file from most word-processing programs (or directly from LOTUS), because it will be too wide (**ISOPLOT** won't have any problems with the file, though). If you want to store just a subset of the calculated data, in order to maintain compatibility with another program, or just to keep the file compact, specify either "Zircon" or "Whole-Rock" format.

The "Zircon" format will contain all of the parameters listed in Table 3 *except*: $^{207}Pb/^{204}Pb$, $^{208}Pb/^{204}Pb$, $^{207}Pb/^{206}Pb$, $^{208}Pb/^{206}Pb$ ratios & errors, the thorium-concentration error, and the $^{238}U/^{204}Pb$-$^{235}U/^{204}Pb$-$^{232}Th/^{204}Pb$ ratios or errors.

The "Whole-Rock" format will contain all of the parameters listed in Table 3 *except*: any of the radiogenic-isotope ratios or errors, and the common-Pb concentration & error.

When you've specified the file format, *PBDAT* will ask for a file-title. This title will occupy the first row of the reduced-data file, and will appear when you access the file from **ISOPLOT**.

PBDAT's reduced-data files are simple ASCII files which can be accessed with any program that can deal with text files, including most word-processing programs. If you want to convert a "Zircon" or "Whole-Rock" reduced-data file from PBDAT into a LOTUS spreadsheet file, though, you can use the macro in the LOTUS file named **PCONVERT.WK1** on the *PBDAT* disk.

To use this macro, retrieve **PCONVERT** from LOTUS, and set the default directory to the path containing *PBDAT*'s LOTUS files. Press **ALT-G** to start the macro. Enter the path and name of the reduced-data file. When the macro pauses and prompts you for another file name, enter a name for the LOTUS-format file (don't include an extension). As soon as the macro has stored this LOTUS-format file, you are ready to press **ALT-G** again to convert another reduced-data file.

Converting a "Complete" format reduced-data file to a LOTUS-format file is more complex. You'll need to split the source-file into two parts with the **SPLIT** program (which accompanies *PBDAT*). **SPLIT** will ask you for the path that the source-file resides on, then the name of the source-file. After some disk-accesses, the program will then ask you for a "root name" for the output files. Whatever name you enter, **SPLIT** will add **L** to the start of the root-name for one of the split files, and **R** to the start of the root-name for the other split file. For example, **QUEER.PRN** would become **LQUEER.PRN** and **RQUEER.PRN**.

Once you've "split" the "Complete" reduced-data file, you can convert it to a LOTUS file with the macro in the LOTUS **CCONVERT** file. The **CCONVERT** macro works just like the **PCONVERT** macro, except that you'll need to enter **2** file-names to specify the source-file. Enter the **L**-file first, then the **R**-file, as created by **SPLIT**.

Once you've created a reduced-data file, if you invoke *ISOPLOT* directly from *PBDAT* (by pressing **ALT-I** from the top-level screen, or from the **FILES** pull-down menu), *ISOPLOT* (versions 2.50 and later) will immediately access that reduced-data file.

USING LabData FILES

LabData files contain the data for a laboratory's spikes, typical blank compositions, and typical mass-discriminations of isotope-ratio measurements (Table 4). If necessary, you can define several **LabData** files for the various spikes or other variables that might be used by your lab.

Defining a New Labdata File

To define a new **LabData** file, select the **Create New** option from the **LabData** menu. *PBDAT* will ask you which spikes you wish to define, and present you with a FORM for each spike. The spike FORMs will require the concentrations (in moles per gram) of the major spike-isotope, the ratios of the isotopes in the spike (these must have already been corrected for mass-discrimination bias), and the uncertainties of the concentrations. If most of your data reduction is for *suites* of samples (where the *relative* concentration-uncertainty is of more relevance than the *absolute* uncertainty), you should assign concentration uncertainties of zero, unless you have significant random errors (such as weighing errors) in your spike delivery.

After you've defined the spikes for the new **LabData** file, *PBDAT* will display FORMs for blanks and for mass discrimination. The BLANKS FORM will require you to enter typical uncertainties (in percent of the amount) for any assigned Pb, U, and Th blanks, as well as the Pb-isotope ratios of the Pb-blank, the uncertainty (absolute this time, not percent) in these ratios, and the correlations of the ratio-uncertainties.

Realistic uncertainties in the blank amounts are typically very high -- 30% to 100% for Pb, and 100% or more for very low U and Th blanks. Also, the correlation between the uncertainties of the Pb-blank 206/204 and 207/204 ratios is generally rather high (0.7-.9), as common leads from random ore deposits (whence comes, ultimately, most of your Pb-blank) in general will have highly correlated 206/204 and 207/204 ratios. This is true also for the 206/204 - 208/204 uncertainty correlation, but to a lesser degree (due to the effect of variable Th/U ratios for the sources of base-metal ore deposits).

The mass-discrimination FORM requires estimates of typical mass-discrimination (arising during measurement in the mass spectrometer) for your Pb, U, and Th runs, in percent per mass-unit[1]. You'll also need to assign uncertainties in your estimates, in absolute values. So if your typical mass-discrimination for Pb runs is 0.11% per mass unit with a possible range (2ó) of from 0.06% to 0.16%, you would enter the uncertainty as 0.05.

Other LabData File Operations

---

[1]Positive values indicate enrichment of the lighter isotopes during analysis.

You can use the **Edit...** option in the **LabData** menu to edit the values for the spikes, mass-discriminations, or blanks of the **LabData** file *in memory*. If you want to store your changes on a disk, remember to select the **Store** option from the **LabData** menu before you exit *PBDAT* or load another LabData file into memory. Use the **Re-Name** option to either rename a LabData file in memory, or to store a modified version under a different name.

Use the **Load New** option of the LabData menu to switch from one **LabData** file to another. You can inspect or print out the values for the LabData file in memory with the **Display** and **Print** options.

COMMON ERRORS IN USING *PBDAT*

There are several common mistakes that users make in using *PBDAT*, usually because of a misunderstanding about exactly what sort of errors should be entered for the various parameters. Some of the more-common errors are:

1) **Using over-optimistic uncertainties for the blank amounts and Blank-Pb isotope ratios.**

It is not at all uncommon for Pb blanks to vary by 50% or more, especially if the procedure or reagents vary over time. The only time a small value, such as 10%, is justified is when that value is the 2ó variation of many (say 5 or more) blanks on an unchanging procedure. The same comments hold for the isotope ratios of the blank. For blanks which are typically very small and difficult to measure (such as for U and Th), the uncertainty can be even larger (a factor of 2 or more).

2) **Using fractionation-uncertainties derived from replicate runs of standards and applying these uncertainties to samples.**

Fractionation uncertainties derived from pure standards (which have not seen any chemistry) generally constrain only the *minimum* fractionation range, as such runs are commonly done in a more-reproducible manner than actual samples. For example, the samples have seen a chemical purification (which, to the extent that it is not perfect, can affect the running behavior of the filament-load); the samples may vary widely in size, whereas the standard runs are generally for a relatively constant amount - thus the standard runs may have been taken at a much more restricted range of filament temperatures than the samples.

3) **Assigning a concentration-uncertainty to the spikes that reflects the *absolute* uncertainty in concentration, rather than the random, sample-to-sample error.**

To repeat what I've said earlier in this documentation: If most of your data reduction is for *suites* of samples (where the *relative* concentration-uncertainty is of more relevance than the *absolute* uncertainty), you should assign concentration uncertainties of zero, except for weighing errors in your spike delivery. If you really want to know the effect of the true spike-concentration uncertainty for an isochron or concordia-intercept age, you'll have to vary the spike concentrations

by what you think the true error might be, re-reduce the suite of data, and re-calculate the regression line for the suite.

4) **Assigning nonzero isotope-ratio uncertainties for the initial-Pb of a suite of samples that probably shared the same initial-Pb.**

This topic is discussed in a note under the discussion of the "Initial-Pb Isotope Ratios" Form.

UTILITY FUNCTION FOR CALCULATING RADIOGENIC ^{207}Pb/^{206}Pb AGES

You can use *PBDAT* as a quick tool for calculating radiogenic ^{207}Pb/^{206}Pb ages by selecting the **Age From Rad. 207/206** option from the **Utilities** menu. Enter the radiogenic ^{207}Pb/^{206}Pb ratio together with the percent error in the ratio (optional) and the time that radiogenic Pb-isotope growth ended (also optional). If the second optional value is not entered, a value of zero is assumed (yielding the usual radiogenic 207/206 age).

UTILITY FUNCTION FOR CALCULATION OF STACEY-KRAMERS MODEL AGES

To calculate Stacey-Kramers (Stacey and Kramers, 1975) single-stage Pb evolution ages and μ-values[1], select the **Stacey-Kramers Model-Age, Mu** option from the **Utilities** menu. Enter the ^{206}Pb/^{204}Pb and ^{207}Pb/^{204}Pb ratios of interest. *PBDAT* will calculate the model age and μ for the specified ratios.

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[1]Ratio of ^{238}U/^{204}Pb normalized for U-decay to the present day.

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INDEX

Table 1: Example of Reduced-Data Output

```
Sample: NZD-45046/a NM10


           206/204   %err        206/207  %err          206/208   %err
UNSPKD    7356.6    1.7         10.254   .0043         14.325    .0054
SPIKED    ---       ---         10.225   .012          2.3446    .0031
SPIKE     16.2                  .3128                  .0000931

BLANK:  6/4=18.9+/-2    7/4=15.55+/-.2     8/4=37.9+/-1.8
 .02537  g Pb208 III     spiked, @ 9.7922E-09 +/-.05%    moles 208/g
 .02774  g U235 III      spiked, @ 5.9419E-08 +/-.05%    moles 235/g
 .02774  g Th230 II      spiked, @ 7.981E-08 +/-.15%     moles 230/g

      SAMPLE WT.    TOTAL-AL.   Pb-UNSPIKED AL.   Pb-SPIKED AL.
       .01234        .74559        .53214            .21345           grams
-------------------------------------------------------------------------
      Pb-Unspiked Aliquot, Corrected for  .065+/- .039 Ng Pb-Blank,
         and  .11+/- .05 % per a.m.u. Mass-Discrimination
   206/207       206/208        206/204        207/204        208/204
   10.246        14.312         7509           732.85         524.67
  +/-.0545%     +/-.127%       +/-2.07%       +/-2.06%       +/-2.03%
 Error-Correls:  207/204-206/204= +.9996598    208/204-206/204= +.9982136

                        Moles Pb per gram:
    206           207            208            204            TOTAL
  1.969E-07     1.9217E-08     1.3758E-08     2.6222E-11     2.299E-07
  +/-.131%
 3.3  Ng Common-Pb in Unspkd Al. ---- ( .369 PPM)
 PPM Total Pb = 47.401        Pb-Spiked Aliquot Blank = .16 Ng
-------------------------------------------------------------------------
238/235 = 5.4376 +/- .014%              232/230= .7537 +/- .032%
 .005 Ng U-Blank,      .008 Ng Th-Blank      U-Th Spiked Al.= .74559 Grams
                         238           235           232
Moles per Gram:     7.6316E-07     5.535E-09     1.358E-07
   182.98    PPM Uranium     (+/-.453%)
   31.51     PPM Thorium     (+/-.62%)                 Th/U= .1722

238/204= 29104                235/204= 211.08   (+/-2.12%)
232/204= 5179                                   (+/-2.16%)
Rho(U/4-6/4)= .975       Rho(U/4-7/4)= .95742      Rho(Th/4-8/4)= .93779
-------------------------------------------------------------------------
TOTAL-PB          206/238        207/235        204/238
 Ratios:          .25801         3.4719         3.436E-05
 Errors:          .472%          .475%          2.12%
 Rho(68-75) = +.9933962    Rho(68-48) = +.2224      Rho(75-48) = +.2395
-------------------------------------------------------------------------
Radiogenic-Pb      206*           207*           208*
Moles per Gram:  1.9648E-07     1.8814E-08     1.2824E-08

Initial-Pb:   206/204= 15.959 +/- .5      207/204= 15.358 +/- .05
              208/204= 35.596 +/- 1       Rho(6/4-7/4) = .7

                206/238        207/235        207/206        208/232

 RATIOS:        .257459        3.39914        .0957547       .094437
 ERRORS:        .472%          .476%          .0614%         .687%
 AGES (Ma):     1476.8         1504.2         1543           1824

 Rho (207/235-206/238) = +.9916304    207/206 Age-Error = 1.2 m.y.
```

Index to LOTUS Column-Positions of Raw-Data Datafile Parameters
For ^{208}Pb or ^{206}Pb - spiked samples

Column	Parameter

C — sample-weight, in grams - actually dissolved

D — weight of solution of dissolved sample before aliquoting

E — weight of Pb-unspiked liquid aliquot of dissolved sample

F — weight of Pb-spiked liquid aliquot   "   "   "

G — grams Pb-spike delivered to F

H — grams uranium spike delivered either to C, D, or F

I —   "   thorium   "   "   "   " "   "

J — unspiked-aliquot ^{206}Pb/^{204}Pb (OR spiked-aliquot ^{206}Pb/^{204}Pb if the unspiked ^{206}Pb/^{207}Pb is unknown and assigned a value of zero)

K — % uncertainty in J (not including mass-discrimination error)

L — unspiked-aliquot ^{206}Pb/^{207}Pb

M — % uncertainty in L (not including mass-discrimination error)

N — unspiked-aliquot ^{206}Pb/^{208}Pb

O — % uncertainty in N (not including mass-discrimination error)

P — Pb-spiked aliquot ^{206}Pb/^{207}Pb

Q — % uncertainty in P (not including mass-discrimination error)

R — Pb-spiked aliquot ^{206}Pb/^{208}Pb

S — % uncertainty in R (not including mass-discrimination error)

T — ^{238}U/^{235}U of U-spiked aliquot (if spiked with ^{235}U), OR

" — Sample-^{238}U/Spike-^{233}U (or ^{238}U/^{236}, if 236 is the spike's most abundant isotope) of U-spiked aliquot (if spiked with U-233/236 and SAM/SPK ratio is used), OR

" — ^{233}U/^{238}U of U-spiked aliquot (if spiked with U-233/236 and SAM/SPK ratio is not used)

U — % uncertainty in T (not including mass-discrimination error)

V — ^{232}Th/^{230}Th of Th-spiked aliquot

W — % uncertainty in V (not including mass-discrimination error)

X — Pb blank of Pb-unspiked aliquot, in nanograms

Y — U blank of U-spiked aliquot, in nanograms

Z — Th blank of Th-spiked aliquot, in nanograms

AA — ^{233}U/^{236}U of U-spiked aliquot (only if SAM/SPK ratio not used)

AB — % uncertainty in ^{233}U/^{236}U   (" "   "   "   " ")

Table 2B

Index to LOTUS Column-Positions of Raw-Data Datafile Parameters
For mixed ^{205}Pb/U/^{230}Th - spiked samples

Column	Parameter

C — sample weight, in grams

D — weight (g) of mixed ^{205}Pb-^{235}U-^{230}Th or ^{205}Pb-^{233U}-^{236}U-^{230}Th spike delivered

E — observed ^{206}Pb/^{204}Pb (not including mass-discrimination error)

F — % uncertainty in E (not including mass-discrimination error)

G — observed ^{206}Pb/^{207}Pb

H — % uncertainty in G (not including mass-discrimination error)

I — observed ^{206}Pb/^{208}Pb

J — % uncertainty in I (not including mass-discrimination error)

K — observed ^{206}Pb/^{205}Pb

L — % uncertainty in K (not including mass-discrimination error)

M — observed ^{238}U/^{235}U ratio (U-spike isotope is 235), OR Sample238/Spike233 ratio (or Sample238/Spike236, if 236 is the most-abundant spike isotope; U-spike isotopes are 233-236 and SAM/SPK is known), OR observed 233/238 ratio (U-spike isotopes are 233-236 but SAM/SPK is not known)

N — % uncertainty in M

O — observed ^{232}Th/^{230}Th

P — % uncertainty in O (not including mass-discrimination error)

Q — Pb blank for Pb run, in nanograms

R — U blank for U run, in nanograms

S — Th blank for Th run, in nanograms

T — ^{233}U/^{236}U of U-spiked aliquot (<u>only if</u> U-spike isotopes are 233-236 and SAM/SPK ratio is not known)

U — % uncertainty in T (if relevant)

V-AB — -- not used for ^{205}Pb-spiked samples

Table 3

Column Headings of Reduced-Data Files ("Complete" Format)

<u>Column#</u>   <u>Heading</u>

1   Sample weight (grams)
2   ppm U
3   ppm Th
4   ppm Pb
5   ppm common-Pb
6   Nanomoles ^{206}Pb per gram
7   Raw ^{206}Pb/^{204}Pb of either Pb-unspiked or Pb-spiked aliquot
8   Blank & mass-discr. corrected sample ^{206}Pb/^{204}Pb (or ^{204}Pb/^{206}P)
9   "   "   "   " ^{207}Pb/^{204}Pb (or ^{207}Pb/^{206}Pb)
10   "   "   "   " ^{208}Pb/^{204}Pb (or ^{208}Pb/^{206}Pb)
11   Radiogenic ^{206}Pb/^{238}U (or ^{238}U/^{206}Pb, or ^{235}U/^{207}Pb)
12   Radiogenic ^{207}Pb/^{235}U
13   Radiogenic ^{207}Pb/^{206}Pb (or ^{206}Pb/^{207}Pb)
14   Radiogenic ^{208}Pb/^{232}Th
15   ^{206}Pb/^{238}U age (Ma) (or ^{235}U/^{207}Pb age)
16   ^{207}Pb/^{235}U "   "
17   ^{207}Pb/^{206}Pb "   "   (or ^{206}Pb/^{207}Pb age)
18   ^{208}Pb/^{232}Th "   "
19   F (^{238}U/^{204}Pb)
20   õ (^{235}U/^{204}Pb)
21   ^{232}Th/^{204}Pb
22   % uncertainty in U   concentration
23   "   Th   "
24   " ^{204}Pb   "
25   " ^{206}Pb   "
26   "   Alpha (^{206}Pb/^{204}Pb) [or ^{204}Pb/^{206}]
27   "   Beta   (^{207}Pb/^{204}Pb) [or ^{207}Pb/^{206}Pb]
28   "   Gamma (^{208}Pb/^{204}Pb) [or ^{208}Pb/^{206}Pb]
29   Error-correlation for Alpha-Beta   [or ^{204}Pb/^{206}Pb-^{207}Pb/^{206}Pb]
30   "   Alpha-Gamma   [or ^{204}Pb/^{206}Pb-^{208}Pb/^{206}Pb]
31   % uncertainty in radiogenic ^{206}Pb/^{238}U [or ^{238}U/^{206}Pb,or ^{235}U/^{207}Pb]
32   "   " ^{207}Pb/^{235}U
33   "   " ^{207}Pb/^{206}Pb [or ^{206}Pb/^{207}Pb]
34   Error-correlation for ^{206}Pb/^{238}U-^{207}Pb/^{235}U [or ^{207}Pb/^{206}Pb-^{238}U/^{206}Pb, or ^{206}Pb/^{207}Pb-^{235}U/^{207}Pb]
35   % uncertainty in radiogenic ^{208}Pb/^{232}Th
35   % uncertainty in Mu and Nu   (^{238}U/^{204}Pb and ^{235}U/^{204}Pb)
37   % uncertainty in ^{232}Th/^{204}Pb
38   Error-correlation for Alpha-Mu   (^{206}Pb/^{204}Pb-^{238}U/^{204}Pb)
38   "   Beta-Nu   (^{207}Pb/^{204}Pb-^{235}U/^{204}Pb)
40   "   Gamma-232/204 (^{208}Pb/^{204}Pb-^{232}Th/^{204}Pb)

Table 4

Example of LabData File Printout

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--------------------------------------------------------------------
DATA FROM LABDATA FILE "ZIRCLAB"

Pb-208 Spike (Pb208 V):
[208] = 1.105E-09 +/- .1  % moles/g
(not a mixed Pb/U spike)
206/204= 17.9         2  0  6  /  2  0  7  =          .  4  2  4  8
         206/208= .0001441

Pb-205 mixed spike  (Pb205a):
[205] = 3.971E-11 +/- .1   % moles/g
[235] = 1.7619E-09 +/- .1  % moles/g
[230] = 1.2909E-09 +/- .1  % moles/g

206/205 = .001128        238/235 = .00612
206/204= 20.33           232/230 = .00243
206/207 = 1.213
206/208= .4846

U-235 spike  (U235 IV):
[235] = 2.3695E-08 +/- .05  % moles/g
238/235 = .007905

Mixed U-233/U-236 Spike  (U233a):
[233] = 4.9584E-09 +/- .1  % moles/g
233/236 = 1.0172      233/238 = 2534

Th-230 spike   (Th230 II):
[230] = 7.981E-08 +/- .15  % moles/g
232/230 = .001292

Average mass-discrimination during mass-spectrometer runs, in %/amu
Pb:  .11 +/- .05       U: .25 +/- .15      Th: .25 +/- .3

Average Blanks:
Uncertainty in assigned amount:  Pb - 60%    U - 100%    Th - 100%
Pb blank ratios and uncertainties:
206/204=18.97+/-1    207/204=15.73+/-.2    208/204=39.18 +/- 1.5
Error-Correlations: 206/204-207/204= .8     206/204-208/204= .7
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