

ISOPLIT VERSION 2

A PLOTTING AND REGRESSION PROGRAM FOR
ISOTOPE GEOCHEMISTS, FOR USE WITH HP
SERIES 200/300 COMPUTERS

by

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INTRODUCTION

ISOPLOT is a program designed primarily for use by isotope geochemists, but of value for anyone who wants to plot X-Y data in a simple, rapid, and flexible manner. Data can be entered either from the keyboard or from data files produced by commercially-available spreadsheet programs. Data can be plotted as a wide variety of symbols, including various error-symbols and polygons. ISOPLOT can regress data using a modification of the most-widely used two-error regression algorithm, and will calculate either isochron ages or concordia-intercept ages directly from the regression lines.

In addition to the basic X-Y plotting and isochron calculation functions, the program can also:

- * construct concordia ($^{206}\text{Pb}/^{238}\text{U}$ - $^{207}\text{Pb}/^{235}\text{U}$) plots and calculate concordia-intercept ages and errors;
- * construct single-stage growth-curves for plots of common-Pb data;
- * construct log-log and semi-log plots;
- * construct plots of REE patterns;
- * calculate and construct plots for weighted averages of a single variable;
- * construct simple histogram plots;
- * calculate useful isotopic functions such as $^{207}\text{Pb}/^{206}\text{Pb}$ ages, common-Pb model ages, Nd and Sr model ages, ages from the secular global-marine Sr-isotope trend;
- * do curvilinear (polynomial) regressions for X-Y data (weighted or unweighted);

- * do least-squares regressions for almost any function using the Simplex method;
- * fit a smooth curve (either precisely or in a least-squares sense) to data of arbitrary complexity using spline curves;
- * manage disk-housekeeping tasks such as disk formatting, file copying, and file packing.

ISOPILOT VERSION 2 is intended to be simple to use, and so is provided with abundant **HELP** screens, extensive error-trapping, and detailed prompts. As a result, most users may seldom need to refer to this manual.

The pedigree of ISOPILOT VERSION 2 extends back several years, starting with programs written in the mid 70's for HP-9830/9831 computers, in the early 80's for HP-86/87 computers (Ludwig, 1983), and most recently for HP Series 200 computers (Ludwig, 1985). ISOPILOT VERSION 2 is an evolutionary improvement on ISOPILOT200, differing mainly in the large number of added capabilities and correction of bugs in the earlier versions.

To obtain disks containing ISOPILOT VERSION 2 (either in HP format or as an ASCII file on MS-DOS format disks), write directly to the author at the address on the cover of this documentation, with the appropriate blank disks enclosed. You may also obtain a printout of the program code, but because of the length of the program, this list will be much less useful than the program disks themselves.

HARDWARE REQUIRED BY ISOPILOT VERSION 2

ISOPILOT VERSION 2 was written for Hewlett Packard Series 200 and Series 300 computers (including the older models 9816, 9817, and 9836). Hewlett-Packard BASIC version 2.1, 3.x, 4.x or later is required to run the programs¹. You should have at least 750 kilobytes of RAM available before loading the BASIC language. The program also requires a printer (assumed to be at address 701) and, if high-quality hard-copy is desired, either an HP-7475 6-pen or HP-7470 2-pen plotter (assumed to be at address 705).

¹A version of ISOPILOT will be available for IBM-PC compatible computers in the late summer of 1988. This version will support CGA, Hercules, and EGA graphics (but not plotter output), and will access data in LOTUS *.PRN files.

If you're using the BASIC 2.1 language, you must have the AP2_1 and GRAPH2_1 extensions in memory. For the BASIC 3.0 or 4.x versions of the language, the required extensions are GRAPH, GRAPHX, MAT, CLOCK, KBD, ERR, KNB2_0, CS80, HPIB, and MS. In addition, if the computer is a Series 300 model, you will need to have the Series 200 Graphics Emulation board installed.

The program assumes that the keyboard is the OPTION 805 (ASCII extended keyboard character set or "Nimitz") keyboard -- the one that's identical to the standard keyboard of the HP-9836. The standard Series 200 keyboard should work with little or no modification, however. Modifications to work with keyboards containing only 8 function keys (softkeys) are being tested.

The programs were developed using a dual single-sided 3.5" disk drive (model HP-9121), but will also work with the HP82905B 5.25" drive and the HP-9122 double-sided 3.5" drive. You won't be able to make the VISICALC spreadsheet program -- used as a data-filer by ISOPLOT -- work with the HP-9122, however, which is a significant disadvantage. It is possible to use the CONTEXT MBA spreadsheet program (similar in its capabilities to LOTUS 1-2-3) with the double-sided drives. Unfortunately, CONTEXT MBA seems to be a more clumsy and hard-to-learn program than HP's implementation of VISICALC. Data files created by the PBDAT200 program (Ludwig, 1985), however, are compatible with all drives.

You can use ASCII files created by other programs. For example, if you have a program that permits you to transfer data on MS-DOS disks to HP-formatted disks (for example, the commercially-available PCLIF program), you can import data from Lotus 1-2-3 .prn files. To do this, you may need to use a second, 5.25" dual-disk drive to permit easy transfer and access to both 3.5" and 5.25" disk drives at the same time.

PRELIMINARY REMARKS ON USING ISOPLOT

First, you should understand some of the basic features of the computer -- the keyboard editing keys (left, right, up, and down arrows), what the softkeys (k0 - k9) are for, and how to answer a query by the program. So if you have the time, you should read the introductory manual to the computer.

If you don't have the time, at least know that: to answer a query, type in your response and press the ENTER KEY (not the CONTINUE or EXECUTE keys); and also that the softkeys are keys whose functions vary according to what the program assigns them. These functions are labeled at the bottom of the CRT in boxes that "map" to the softkeys

themselves.

If you're not sure which softkey to press to get the program to continue after it has completed some operation, try pressing the **CONTINUE** key. The program will then select a logical action to take, based on the assumption that you didn't want to do anything complicated.

ISOPLOT tries to allow you to gracefully back out of most of the situations that you might mistakenly stumble into. The most common way exists whenever you see that softkey **k9** is labeled **ESCAPE**. Just press this **ESCAPE** softkey, and the program will back up at least one level--probably to where you were before you made your error.

If an **ESCAPE** softkey doesn't exist and the program is asking you to enter a response to a query, you can still usually back out by entering an asterisk as your response. If neither the **ESCAPE** softkey nor an asterisk response is available, you can still regain control by pressing the **PAUSE** key, then the **RUN** key. This method will re-start the program and re-set all its defaults, however.

If the program is hung up, perhaps it's the fault of the printer or plotter. Try pressing the **CLR/IO** key, fixing the problem, then pressing the **CONTINUE** key.

If all else fails, please pay attention to what the CRT is asking you to do! Your chances of misunderstanding what the program expects will be greatly increased if you ignore the specific wording of the queries and prompts. If you're still at sea after examining the CRT, see if it indicates that there is a **HELP** screen available (via either a **HELP** softkey or by pressing **CTRL H**). In fact, in your initial encounters with **ISOPLOT**, it's a very good idea to invoke every **HELP** screen that you come across, unless you want to spend a lot of time re-reading this manual. The **HELP** screen information is stored on the same disk as the program, so you'll need the **ISOPLOT** disk present in either one of the drives.

GETTING STARTED

LOADING THE PROGRAM

To load the program first make sure that the **BASIC** language and the required extensions already reside in memory. Put the **ISOPLOT**-

MAIN disk¹ in the left-hand drive and type in **LOAD "ISOPLOT:,700,0",1**. The program will take about a minute to load and begin running. If you intend to use either the **HELP** screens (which you should) or one of the auxiliary sub-programs of **ISOPLOT** (these include routines for histogram plots, polynomial fitting, spline-curve fitting, Simplex-method curve fitting, marine Sr-isotope ages, and file repacking), you should put the **ISOPLOT - AUXILIARY** disk in the other drive. After **ISOPLOT** is loaded, you can remove the **MAIN** disk if you wish.

SETTING UP THE PLOT (X-Y plots)

The first CRT-display of the program will look something like this:

Rev. Jan. 22, 1987 536 Kbytes avail. K.R. Ludwig, U.S. Geol. Survey
 <<<<<<<<< ISOCHRON or X-Y PLOTTER >>>>>>>>

CRT PLOT	E Change <u>E</u> rror format or Customize tick-intervals C Start a <u>C</u> oncordia plot A Start a <u>W</u> eighted <u>A</u> verages plot H Start a <u>H</u> istogram plot R Start an <u>R</u> EE plot L Select <u>L</u> inear, <u>L</u> og, or <u>L</u> og-Log X-Y axes V Run <u>V</u> ISICALC F <u>F</u> ormat/Initialize a disk D <u>D</u> uplicate/copy files from a disk 1 calculate a 207/206 age 2 calculate a model-Pb age 3 calculate a model-Nd age 4 calculate a model-Sr age	CRT OUTPUT
----------	--	------------

errors are 2-sigma, in percent

PRINTER OUTPUT	PLOTTER PLOT			HELP
			GET DATAFILE	START

¹If you are using either a hard-disk drive or a double-sided 3.5" drive, I suggest that you combine the files on the **MAIN** and **AUXILIARY** disks onto one disk, using the **COPY** command or the file-copying utility of **ISOPLOT**.

In this section, I'll discuss the use of the ISOCHRON or X-Y PLOTTER functions. If the display says anything else but this, press the I key to revert to the X-Y Plotter functions; if the display shows PLOTTER PLOT at the upper left, press k1, and if it shows PRINTER OUTPUT at the upper left, press k0.

First, select where your plot and alphanumeric output are to be sent. Softkey k0 determines whether the alphanumeric output is to be sent to the printer or to the CRT, and toggles between the two. Look at the upper right of the CRT to see what the current status is. Notice that the k0 label will always be the opposite of the status display. This is because the softkey labels indicate what the softkey will do when pressed, not what the current status is.

Next, select where you want the plot to appear -- on the CRT or the plotter (I suggest that you always put your first version of a plot on the CRT and do your debugging there -- it's much faster). The current plotting device is shown at the upper right of the CRT. Use softkey k1 to toggle between using the CRT and using the plotter.

If you select the plotter as the plotting device, several more softkeys, along with other information, will be labeled towards the bottom of the CRT, as shown below:

Errors are 2-sigma, in percent
Single Lines

Pen-Speed=9

Relative Label-Size=1
Use Pen# 1

PRINTER OUTPUT	CRT PLOT	CHOOSE PEN	STACKED PLOT	HELP
ADJ. LABELSIZE	DOUBLED LINES	PEN SPEED	GET DATAFILE	START PLOT

To select one of the 6 pens of the plotter, press k2. One of the bottom lines of the CRT will then instruct you to choose a pen by pressing the number-key corresponding to the pen you want.

To specify the pen speed (how fast the pen moves while drawing lines and characters), press k7. Use the fastest speed (9) for draft plots, slower for final plots. The default speed is the fastest.

To vary the relative sizes of the axis and tick labels of the plot (plotter plots only), press k5.. The default size of 1 is suitable for plots that will not be reduced very much during reproduction, but

larger sizes (up to 2 or so) are best for plots that will be made into 35mm transparencies or reduced to fit into journals.

If you want your plot drawn with thicker, bolder lines than normal, press **k6** (**DOUBLED LINES**). The plot will then be drawn twice, with the lines slightly offset the second time.

If you want to stack plots so that they share the same X-axis (and X-axis limits), construct the lower plot as usual, but with specifically-defined limits for the plot-box (see below). Then for the upper plot, press **k3** (**STACKED PLOT**). Position the plot-box precisely over the lower box (that is, with the same specifications for the X-locations of the box - again, see below). Because you specified a **STACKED PLOT**, the upper plot will be drawn without labels for the X-axis and without a label for the lowermost tick of the Y-axis. Figure 3 shows an example of a stacked plot.

Notice that at the lower left of the starting CRT-display there is a message indicating the error-format that will be assumed by the program. The default format is for errors to be entered in percent, and at the 2-sigma (or 95%-confidence) level. You can change the assumed error-format, though, by pressing **E** from the starting display. Optional error-formats include absolute (rather than percent) errors, and 1-sigma rather than 2-sigma errors.

Semi-log and Log-Log Plots: -- You can have either the X-axis, the Y-axis, or both axes be plotted logarithmically (figure 4) by invoking the Logarithmic/Linear Axes option from the starting display (press **CTRL L**). To revert back to linear axes, invoke the same option again. Remember that all values to be plotted logarithmically must be greater than zero.

Choosing the Axis Names: -- When you've finished selecting the physical parameters of the plot with the softkeys, as described above, press the **START** softkey (**k9**). The CRT display will then be:

...Use ^ to start superscripts or end subscripts,
* to start subscripts or end superscripts.

ENTER X-AXIS NAME, Y-AXIS NAME:

(press CONTINUE to use PPM Sr and PPM Rb)

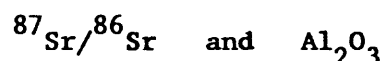
Or press a softkey for these common isotopic plots:

<u>k0</u> -- Pb 206/204-207/204	<u>k4</u> -- Sm-Nd isochron
<u>k1</u> -- Pb 206/204-208/204	<u>k5</u> -- 238/204-206/204
<u>k2</u> -- Pb-204/206-207/206	<u>k6</u> -- 235/204-207/204
<u>k3</u> -- Rb-Sr isochron	<u>k7</u> -- 232/204-208/204

Pb 6/4-7/4	Pb 6/4-8/4	Pb 4/6-7/6	Rb-Sr	Sm-Nd
Mu-Alpha	Nu-Beta	Th/204-Gamma		ESCAPE

The axis names are the names that will be labeled under the X-axis and to the left of the Y-axis. You can respond to the query in 3 different ways: (1) by typing in the X-axis and Y-axis names, separated by a comma, and pressing the ENTER key; (2) by pressing CONTINUE to re-use whatever names were used for the last plot or used by the last-loaded data-file (PPM Sr and PPM Rb in the above example); or (3) by pressing one of the softkeys to select one of the "standard" radiogenic-isotope isochron plots.

You can specify superscripts or subscripts in the axis names by using the ^ symbol to bump the following characters up a third of a line, and the * symbol to bump the following characters down a third of a line. So if you wanted the axis names to look like



you would enter the names this way:

$^{\wedge}87^* \text{Sr} / ^{\wedge}86^* \text{Sr} \quad \text{and} \quad \text{Al}^*2^{\wedge}0^*3$

NOTE: If you actually want to use the asterisk and caret symbols in the axis names, you can do so by using CTRL ^ and CTRL * instead of ^ and *.

Entering the Plotbox Limits: -- After you've entered the axis names for the plot, the CRT will display:

ENTER X AND Y LIMITS ([Xmin,] Xmax, [Ymin,] Ymax)?

(press CONTINUE to re-use 0, 14, .7, 1.2)

(press k0 to get plot limits from datafile data)

Your response to this query defines what the minimum and maximum X- and Y-values of the plotbox will be. You can enter just 2 values, in which case the X and Y minimum values will be assigned values of zero; or you can enter 4 values if at least one of the minimum limits is nonzero. If you just want the same limits as were used for the last plot, though, just press CONTINUE without entering any values. At this point, if your plot is to be drawn on the CRT, the program will construct the plot box, tick labels, and axis labels.

If data from a datafile were already loaded into memory when the above CRT-display appeared, you could request that the program decide the plot limits: just press the AUTOSCALE softkey (k0). The plot limits will then be selected to include all of the values present in the datafile.

The format for entering values in response to a query by ISO PLOT is similar to the above example throughout the program. Values for prompts in brackets are optional -- a default value will be used if you don't enter a number for them. To enter several values at once (as indicated in the prompt), just separate the values by commas. And, for many queries, there is a default value or set of values that will be assumed if you just press the CONTINUE key without typing in any response. These default values will be included in the prompt.

The program will automatically calculate the best tick-intervals for the X- and Y-axes, and adjust slightly your specified limits so that they fall precisely on a tick interval. You can over-ride these adjustments if necessary, though. To do so, see the section on What If the Default Limits and Ticks are Unsatisfactory?.

Defining the Physical Size of the Plot: -- If you requested that your plot be drawn on the plotter (rather than the CRT), you'll have to specify the size of the plot. The CRT query will be:

ENTER PLOT-SIZE (3-10)

Press CONTINUE default size of 8)

(press k4 for nonstandard dimensions/locations)

Centered plots: If you want a plot with a "normal" height-to-width ratio (about the same as an 8.5" by 11" sheet of paper) and centered in the paper, enter a number from 3 to 10 in response to the above query. A value of 10 gives the largest plot that will fit on an 8.5" by 11" sheet of paper, and a value of 3 gives a plot only about 30% as large. Intermediate values give proportionately intermediate sizes. The default size is 8.

Uncentered plots: If you want a plot with a different height-to-width ratio (perhaps only 5 cm high by 10 cm wide), or located off-center in the paper, press k4. The CRT will then display:

**PRESS k0 TO DEFINE THE PLOT-LIMITS FOR THE ENTIRE FIGURE AREA,
k4 TO DEFINE LIMITS FOR THE PLOT-BOX ONLY**

If you want to define the area that the total plot will occupy, including tick-labels and axis names, press k0. If you want to specify the location and area of the plot in terms of the plot box, however (the plot box is the box with ticks outlining the area where the data points are actually plotted), press k4. The latter option is particularly useful when you are putting two or more plots on the same piece of paper, and is essential if you want to stack two plots (see the **STACK PLOT** option above) that share the same X-axis and X-limits.

Entering the plot limits: Once you've selected how you want to define the location and size of the plot, the CRT will query:

ENTER PLOT-LIMITS IN mm: X-MIN, X-MAX, Y-MIN, Y-MAX?

(max. limits are 0-249 [X] and 0-179.5 [Y],
lower-left corner of paper is 0,0)

Enter 4 values, separated by commas, to define the location of the X-limits of the plot (X-MIN, X-MAX) and the Y-limits of the plot (Y-MIN, Y-MAX). The lower-left corner of the paper is defined as X=0, Y=0. Enter your values in millimeters. The program will now start to draw your plot.

What if The Default Limits and Ticks are Unsatisfactory? -- If you need to specify precisely the maximum and minimum X- and Y-values of the plot box and the axis-tick intervals, you can force ISOPLOT to accept your specifications by invoking the CUSTOM TICKS option. To do this, press E from the starting screen, then softkey k5 (CUSTOM TICKS). The screen will clear and display:

CUSTOM TICK SPECIFICATION

This option allows you to specify the X- and Y-limits and the X- and Y-tick intervals without having ISOPLOT over-ride your choices.

REMEMBER that the maximum X- and Y-values will still be forced to lie precisely on a tick.

You can also specify the Concordia tick-interval, which tick will be the first to be labeled, and up to 4 concordia ticks which will not be labeled.

Enter the desired X & Y tick intervals, separated by a comma...
(press CONTINUE to just enter values for the concordia ticks)

Enter 2 values: the desired X-tick and Y-tick intervals. You'll be asked to enter the axis limits later. Be careful to have neither too many nor too few ticks on your axes -- about 8 to 16 ticks is the normal range.

The above example shows you the screen you will get for a Concordia plot; for just X-Y or isochron plots, there will be no mention of Concordia ticks. But if the plot is a Concordia plot (see CREATING CONCORDIA PLOTS), after you enter the axis tick-intervals, the program will display:

Enter the Concordia tick-interval, 1st labeled tick, Labels to be skipped (Ma)?

(Enter 2 to 6 values, separated by commas; CONTINUE to accept default values)

You can enter from 2 to 6 values, or accept the program's usual default values by just pressing CONTINUE. The first two values must be the desired tick interval for the Concordia curve, in millions of years, and the value of the first (youngest age) tick that you want labeled. Obviously, this second value must be an integral number of tick-spacings from the first value.

The third to sixth value(s), if any, must represent the values of Concordia ticks that you don't want labeled. This can be useful, for example, if you know that data points or a regression line will interfere with a tick label.

PLOTTING DATA-POINTS

THE SELECT PLOTTING-SYMBOL SCREEN

After the program has drawn the plot box, tick labels, and axis names, you're ready to start plotting your data. First, though, you must select a plotting symbol. The CRT display will be:

SELECT A PLOTTING SYMBOL TO PLOT DATA

press CTRL L to draft a phrase on the plot

press CTRL P to dump the plot to the printer

press CTRL D to dump the plot to the plotter

press CTRL ^ to connect-the-dots

press CTRL H for HELP

press any key for keyboard plotting-symbol

ERROR BOX	ERROR ELLIPSE	ERROR CROSS	POLYGON	OPTIONS
SOLID LINE	CHOOSE PEN	YORKFIT	GET DATAFILE	NEW PLOT

I'll refer to this display as the SELECT PLOTTING SYMBOL display. The bottom rows show the softkey definitions.

You can do several things from this part of the program besides just selecting a plotting symbol, but for now we'll ignore them. The simplest type of plotting symbol to use is just an alphanumeric symbol such as + * X 0 or A H 5 #. To specify such a symbol, just press the corresponding key (if you want to vary the size of alphanumeric symbols, you can do so from the OPTIONS screen). As soon as you specify a symbol, the program will ask you for the data to be plotted.

POLYGON PLOTTING-SYMBOL

You can use a polygon for a plotting symbol, with any number of sides, size, and rotational orientation, either open or filled. Press the softkey labeled POLYGON (hold down the SHIFT key also if you want a filled polygon). The CRT will then query:

POLYGON SYMBOL: ENTER #SIDES (- for star),
[,SIZE (mm) [,ROTATION (0-360)]]

Press CONTINUE to re-use last values (20,2.5,0)

As usual, the parameters in brackets represent optional input, so you can enter either 1, 2, or 3 values (or press CONTINUE to specify the values that were used last). The number of sides can vary from 3 (a triangle) to a large number (anything over 20 will give a circle). The SIZE parameter refers to the diameter of the polygon in millimeters; default is 2.5. The ROTATION parameter refers to the angular orientation (counter-clockwise from the X-axis) of a vertex of the polygon: 0 gives a vertex at 3 o'clock, 45 a vertex at 1:30, 90 a vertex at 12:00 and so on. The default value depends on the number of sides of the polygon, and gives what I have decided are "conventional" orientations (triangle pointing straight up, square with sides parallel to the X and Y axes, pentagon pointing straight up...).

If you enter the number of sides of the polygon as a negative value, the polygon will be drawn "puckered in" at each side, so the result is a "star"-shaped figure (figure 1). For example, if you specified the number of sides as -5 instead of just 5, the plotting symbol will be a 5-pointed star.

PLOTTING SYMBOLS THAT INDICATE ERRORS

There are 3 plotting symbols that you can use to indicate the errors of the points on the plot: error box, error cross, and error ellipse. If you select one of these symbols, the program will need estimated errors for each of the data points. If you select the error ellipse symbol, the program will also need values for the X-Y error correlations. If you don't know how to estimate an error correlation, use this equation:

$$\text{Rho} = (E_x^2 + E_y^2 - E_z^2) / (2E_x E_y)$$

or:

$$E_z^2 = E_x^2 + E_y^2 - 2E_x E_y \text{Rho}$$

where Rho is the correlation between the X and Y errors, E_x , E_y , and E_z are the percent errors in X, Y and Z, and where $Z=Y/X$. For example, if X were $^{206}\text{Pb}/^{204}\text{Pb}$ and Y were $^{207}\text{Pb}/^{204}\text{Pb}$, then Z would be $^{207}\text{Pb}/^{206}\text{Pb}$. Or, if X were $^{207}\text{Pb}/^{235}\text{U}$ and Y were $^{206}\text{Pb}/^{238}\text{U}$, then Z would be $R \cdot ^{207}\text{Pb}/^{206}\text{Pb}$ ($R = \text{natural } ^{235}\text{U}/^{238}\text{U}$). Error correlations are zero if the error in Y doesn't tend to increase with the error in X. If the error correlations are much greater than about 0.5, don't use error box or error cross symbols, because these symbols will convey a misleading impression as to the actual area of uncertainty around the data point.

To use an open error box or error ellipse, just press the appropriately-labeled softkey. To get filled symbols, hold down the SHIFT key while pressing the softkey.

ENTERING DATA FROM THE KEYBOARD

As soon as you select a plotting symbol, the CRT will clear and display:

PLOTTING SYMBOL IS * (data-values of zero not accepted)

2-SIGMA %-ERRORS

INPUT DATAFILE SET #S AS 1st SET, LAST SET-ASTERISK

(e.g. 2.12* or 2.12;15.18*)

[use *L or *R to label data-file name to (L)eft or (R)ight of point]

set#	87Rb/86Sr	%err	87Sr/86Sr	%err	RHO
------	-----------	------	-----------	------	-----

#1: 87Rb/86Sr, [%err,] 87Sr/86Sr [,%err] [,-err-corr.]
(CONT WHEN DONE)

The axis names and plotting symbols shown above are only examples, of course.

To enter the X- and Y-values for your data points, just type in the two numbers, separated by a comma, then press the ENTER key. To include the errors with the points (necessary for plotting symbols that reflect errors or for Yorkfits), enter 4 values separated by commas, in the format X, X-error, Y, Y-error. The default error-format is for errors to be entered in percent and at the 2-sigma level (but you can change this). If no error correlations are entered (as the optional 5th value), they are assumed to be zero. If the errors for all of the points are going to be the same, don't bother entering them at this point -- you can enter them as a group later.

When you've entered all of the points that you want plotted with the particular plotting-symbol or pen color that you have chosen earlier, press CONTINUE. If you're using an error-symbol (error box, error cross, or error ellipse) as the plotting symbol and you didn't enter values for some or all of the errors, the CRT will query:

ENTER X-%err, Y-%err, [,Err.-Corr.] FOR SETS WITH ZERO ERRORS?

Enter the values requested. Note that, again, the error correlation is an optional value, and also that the assigned errors must be nonzero.

The computer will then display a list of the data-point values that you just entered, and query:

SET TO BE CORRECTED? (CONTINUE IF OK)

Check the displayed list for errors, and if you made any, enter the set# (shown to the left of the X- and Y-values) of one of the incorrect data-points. Enter the correct values, when requested, then continue with the editing process until all of the values are correct. Press CONTINUE, and the data points will be plotted.

THE ADD POINTS SCREEN

After the data points are plotted, this display will appear on the CRT:

PRESS GRAPHICS TO VIEW PLOT, ALPHA TO VIEW THIS SCREEN

- " ADD TO INCLUDE THESE POINTS WITH OTHERS FOR A YORKFIT
- " DELETE TO DELETE POINTS FROM THE LAST SET
- " NEW POINTS TO PLOT A NEW BATCH OF POINTS
- " YORKFIT FOR A YORKFIT
- " CTRL E TO DRAW THE ERROR-ENVELOPE FOR THE LAST YORKFIT LINE
- " CTRL ^ TO CONNECT-THE-DOTS
- " POLYNOMIAL TO FIT A POLYNOMIAL CURVE TO THE DATA
- " NEW PLOT TO START A NEW PLOT

(press NEW POINTS if you just want to return to the data-entry screen)

At this point, you can choose to plot more points, do a Yorkfit, or abandon the current plot and start a new one. If your plot is on the CRT, you can toggle between the graphics display and the alphanumeric display (shown above) with the GRAPHICS and ALPHA keys at the upper-right of the keyboard. If you press the NEW POINTS softkey, the program will return to the SELECT PLOTTING SYMBOL display, and any additional data-points that you enter will be counted as a new batch for any subsequent regressions.

But if you want to plot more points (perhaps with a different plotting-symbol or pen color) that are to be pooled with the just-plotted points for a later Yorkfit (or other regression). press the ADD POINTS softkey.

If you don't want to include (for subsequent Yorkfit or other regressions) one or more of the points that you just plotted, press the DELETE softkey. The CRT will ask you which point to delete.

CONNECTING DATA POINTS WITH A LINE

You can connect each data point on your plot with a straight line by invoking the "Connect-the-dots" function from the ADD POINTS screen (press CTRL ^). The data points will be connected from the smallest X-value to the largest X-value.

(cursor or pen at the lower right of phrase) or centered (cursor or pen at the lower center of the phrase) by pressing k6 or k7, respectively.

For left-justified phrases on plotter-plots, you can define the angle from the horizontal of the phrase by using the KNOB to move the pen close to a line or trend on the plot whose angle you want to match, pressing k1 (ANGLE POS.#1), then moving the pen to any second point along this trend and pressing k2 (ANGLE POS.#2).

If you want to start a phrase at a specific X-Y location on the plot, you can specify this location by pressing k0 (ENTER X-Y). When you've positioned the pen, selected the angle (if non-horizontal), and specified CENTER or FLUSH RIGHT (if required), press k4 (ENTER PHRASE) and enter the phrase that you want drafted.

For left-justified phrases, you can specify superscripts or subscripts in the phrase in the same way as the axis labels, using the ^ and * characters. To get a \pm symbol, use +/- . To indicate a "line-feed/carriage-return" (that is, continue lettering down one line and at the original x-location), insert the CTRL L character.

You can change the pen-color in the middle of a phrase by pressing CTRL 0 through CTRL 6 at the positions in the phrase where you want the pen to change. A pen# of zero specifies no pen (so you can see if the position of the phrase will be roughly where you want it).

IDENTIFYING DATA POINTS ON A PLOT

If you have plotted a lot of data points from a data file, you may occasionally find it useful to be able to quickly determine the identity of one or more plotted points. Perhaps, for example, there is an outlier that you suspect may be due to a typographical error in the data table. To identify such a point, follow the procedure below.

- 1) Invoke the LETTER function by pressing CTRL L from the SELECT PLOTTING-SYMBOL screen or from the ADD POINTS screen. Then, enter any number in response to the "CHARACTER HEIGHT" query.
- 2) Turn the KNOB to move the cursor (CRT plots) or the pen (plotter plots) to the unknown point. For CRT plots, you may want to first press SHIFT-CLR LN (in the upper-right region of the keyboard) to clear the distracting messages so that the plotted points are not obscured. You don't have to put the pen or cursor precisely on the point -- just close enough so that no other point is nearer to the pen or cursor.

- 3) Press the WHICH POINT? softkey (k3). The name and set number of the datafile-set closest to the pen or cursor will then appear towards the bottom of the CRT. To identify another point, just move the pen or cursor to it and press WHICH KEY? again.

STORING AND RETRIEVING DATA FROM DATA FILES

You can use the commercially-available VISICALC or CONTEXT MBA programs¹ to construct, edit, and store datafiles that can be read by the program (except when using the Rare-Earth Element Plot option). The VISICALC or CONTEXT MBA data files must conform to a specific format to be read by ISOPLOT, however. This format requires that:

- 1) the column-width be 9 characters (the VISICALC default);
- 2) the column names must appear above any data, and directly overlie a line of repeating equals-signs (=====);
- 3) the column names may occupy up to 2 cell above the repeating equals-signs;
- 4) the first 2 columns (A and B) can be used for sample names only;
- 5) no more than 50 columns are allowed (the maximum number of rows varies from 50 to 500, depending on how much memory you have in your computer);
- 6) the first row of the spreadsheet can be used as a file title (up to 80 characters) to identify the file;
- 7) the file must be stored as an ASCII file (using /PF from VISICALC);
- 8) the file must be stored while the PRINTER WIDTH is defined as 80;
- 9) the file name (as stored on the disk) can include only the characters A through Z (upper-case or lower-case) and numbers 0 through 9.

¹Or even LOTUS 1-2-3 if you have a program for converting MS-DOS disks to the Hewlett-Packard format. PCLIF, a commercially-available program, is one such program.

You can include a column in the VISICALC file that specifies both the pen-number and the plotting-symbol to be used for plotting each point. The column with the plotting symbol and pen number specifications must have the word **SYMBOL** in its column name (column heading) so that the program can recognize its existence.

To indicate a plotting symbol of *, +, O, or X, use the corresponding character as the first one in the cell in the appropriate row and in the plotting-symbol column. Indicate a solid or open error-ellipse symbol with E or e, respectively; a solid or open polygon with P or p. Indicate the pen number with the underscore symbol, then the pen number. For a polygon symbol, after the p or P add the number of sides, size, and rotational angle, separated by commas. For example, to indicate that a data point is to be plotted with pen-number 6 using an open, 7-sided polygon that is 5 millimeters in size with a vertex at 42 degrees, the plotting-symbol cell would contain the characters p7,5,42_6.

When you plot data from a datafile that contains a plotting-symbol column, any data from a row for which a plotting-symbol specifier exists will be plotted with the specified symbol and pen-number (unspecified parameters of the plotting symbol, such as the pen number, will be given default values). The plotting-symbol specifiers will over-ride any input that you may have provided at the time of actually plotting the data.

If you have a translating program that will allow you to convert IBM-PC compatible files to HP compatible files (such as the commercially-available PCLIF program), you can use LOTUS 1-2-3 ASCII (.PRN) files with ISOPLOT. Make sure that you use the file format described above for VISICALC files, and also that you leave the LOTUS left-margin at its default value of 4.

If you're going to do a lot of work with data files, you'll need to know how to format disks and copy files from one disk to another. These topics are covered in the section on *UTILITIES FOR DISK-FILE MANAGEMENT*.

ACCESSING DATAFILES

To get data from a datafile, press the softkey labeled GET DATA-FILE from either the starting display or the SELECT PLOTTING SYMBOL screen. The CRT will then show:

CATALOG Drv #0	CATALOG Drv #1	HELP	PRINT DATA	LOAD DATAFILE
PRINT FILE	ZEROES OK		SCRATCH FILE	ESCAPE

To access data from a datafile, if you're sure of its name, press k4 (LOAD DATAFILE). If you're not sure of its name, or if you want to see what datafiles are present on a disk, press either k0 or k1 (CATALOG). The screen will then show the names of all of the ISOPLLOT-compatible files on that disk¹. You can choose one of these files by just entering the number of that file, as shown on the screen.

Once you've chosen a datafile to access, the computer will search for and display a list of all of the column-names (column headings) for that file. You must then select either 2 columns (X and Y; or, if doing weighted averages, Y and Y-error), 4 columns (X, X-error, Y, Y-error), or 5 columns (X, X-error, Y, Y-error, X-Y error-correlation). If the plot is a Concordia plot, however, ISOPLLOT may be able to select the appropriate columns itself by examining the column names. Also, if the datafile were created by PBDAT200, you can select the appropriate columns for a variety of commonly-used Pb-U-Th isotope plots by simply pressing the appropriately-labeled softkey.

ISOPLLOT will then retrieve the data from the disk, and either display the data on the screen or, if you had pressed PRINT DATA (k3) before loading the file, print out the data. Normally, only nonzero data from the datafile will be plotted. If you want to plot data with either X- or Y-values of zero, you have to press the ZEROES OK softkey (k6) from the GET DATAFILE menu before accessing the datafile. Once you have specified ZEROES OK, all data can be plotted, including data for "empty" cells in the spreadsheet, which are counted as values of zero.

If you just want to examine the data in a file, or to print out the data for more than 5 columns to keep as a record of its contents, press the PRINT FILE softkey (k5). You can then specify up to 14 columns of data to be printed out, in any arrangement. The print size will be automatically compressed if necessary, so that all of the specified columns will fit on a single sheet of paper.

¹You can get a catalog of all of the files on a disk (including program files and ISOPLLOT-incompatible data-files) by pressing SHIFT-k0 or SHIFT-k1.

It can be useful, in many cases, to specify that the datafile data be printed out on the printer the first time you access the file, even if you already have a printout of the file from VISICALC. The ISOPLLOT printout of the datafile will contain the set-numbers assigned to each data-containing row of the file, so that when you specify that a particular subset of the data be plotted, you'll have a record of which set numbers to specify.

USING DATA FROM DATAFILES

To plot from a datafile, you need only refer to the data by "set numbers", where the set number of a data point corresponds to its row in the spreadsheet, and is printed out when the datafile is first accessed by the program. For example, after you've selected a plotting symbol, the screen will show:

PLOTTING SYMBOL IS ERROR ELLIPSE

2-SIGMA ~~3~~-ERRORS

INPUT DATAFILE SET #S AS 1st SET, LAST SET-ASTERISK

(e.g. 2,12* or 2,12;15,18*)

[use *L or *R to label data-file name to Left or Right of point]

To plot the data for set number 5, enter 5*. To plot data for sets 5, 6, 7, 8, and 9, enter 5,9*. To plot data for sets 5, 6, 7, 8 and 11 and 15, 16, 17, enter 5,8;11;15,17. In other words, indicate continuous sequences of sets with a comma, separate different continuous sequences (or individual sets) with a semicolon, and always add an asterisk at the end. It's OK to mix data from datafiles and typed-in input.

You can have the computer label each point with its sample name (from columns A and B in the spreadsheet) by adding an L or R after the asterisk. An added L will give sample names labeled to the left of the point, R will give names labeled to the right of the point. You'll have to deal with any problems of over-writing that this causes.

If you want to plot all of the data in the datafile already in memory, press k8 (ALL POINTS).

Using Keyboard-Entered Data as a Temporary Datafile: -- If you're entering data points from the keyboard, and would like to temporarily "file" those data-points for subsequent re-plotting (perhaps you didn't get everything perfect the first time?), you can do so in the following way. First, press the GET DATAFILE softkey from either the starting screen or the SELECT PLOTTING SYMBOL screen. If the resulting display says that there is currently a datafile in memory, press the SCRATCH FILE softkey. ESCAPE from this

screen.

With no datafile in memory, each data point that you enter is added to a temporary datafile, in the sequence that you enter the points. Only the last batch of data that you entered will be saved, so the temporary file will consist only of N points, where N is the highest set-number entered. In other words, if you type in the X-Y values for 20 points, then press the NEW POINTS softkey and type in another 10 points, the temporary file will consist of the second set of 10 points plus the last 10 (set #s 11 through 20) of the first-entered points.

To re-plot these points, just treat them as points in an ordinary datafile, with set numbers of 1 through 20.

YORKFITS OF DATA

YORKFIT "MODELS"

A "Yorkfit" refers to a linear regression using the general algorithm developed by Derek York (York, 1969). This algorithm weights each point according to both its X- and Y-errors, and also takes into account the X-Y error-correlations. ISOPLOT uses both the original York algorithm, and also a few modifications, depending on the type of data that you are working with and the amount of scatter that the data shows about the regression line. Each of these modifications, called MODELS by the program, makes different assumptions about the reason for the scatter of the points about a straight line.

MODEL 1 Yorkfits: -- The MODEL-1 Yorkfit is York's original algorithm, and assumes that the only cause for scatter from a straight line is the errors that you have assigned to the points. The points are therefore weighted proportional to the inverse-square of these errors. A test of the MODEL-1 assumption is provided by the **PROBABILITY OF FIT** value calculated by the program. If this value is reasonably high (more than 15% to 20%), then the MODEL-1 assumptions are probably (but not certainly) justified. If this probability is low (less than 20% or so), however, you may choose another model. The MODEL-1 errors are calculated using the maximum-likelihood algorithm of Titterton and Halliday (1979).

If you select the MODEL-1 fit even though the **PROBABILITY OF FIT** is low, you are in effect requesting that the actual errors be calculated from the observed scatter (thus invoking the use of the Student's-t multiplier to convert from estimated errors to 95%-confidence errors), and you are also accepting an assumption that the true errors of the data points are directly proportional to the ones you have assigned to them.

ISOPLOT will always attempt a MODEL-1 fit first. In the printout, the A PRIORI errors are the errors in the slope and intercept calculated by propagating only your assigned errors for the points; no matter how much the points scatter, the A PRIORI errors will not increase. The INCLUDING SCATTER errors, however, are calculated from the actual scatter of the points from a line, and are independent of the assigned errors. These errors, given at the 1-sigma level, are provided mainly for comparison purposes with the output of other, simpler implementations of York's algorithm. The only useful errors are the ones given as 95% CONFIDENCE-LIMIT errors.

How the 95% confidence-limit errors are calculated depends on the probability that the assigned errors for the points can account for the observed scatter. If the probability is greater than 0.15, the 95% confidence-limit errors are simply 1.96 times the A PRIORI errors (1.96 is the Student's-t value for an infinite number of points -- the reason for this is discussed by Brooks and others, 1972).

MODEL-2 Yorkfits: -- A MODEL-2 Yorkfit assigns equal weights and zero error-correlations to each point. This is probably seldom justified by any real mechanism, but at least avoids the mistake of weighting the points according to analytical errors when it is clear that, in fact, some other cause of scatter is involved. The 95% confidence-limit errors are calculated from t times the INCLUDING SCATTER errors.

MODEL-3 Yorkfits: -- A MODEL-3 Yorkfit assumes that the scatter is due to a combination of the assigned errors plus a normally-distributed variation (of unknown magnitude) in the Y-values. This model (which is similar to the Model-3 algorithm of M^CIntyre and others, 1966) may be realistic in the case of Rb-Sr and other isochron data for rocks whose initial ratios were variable. For this model, the program will solve for the unknown Y-variation as well as for the best-fit line, so you can judge whether or not the solution is realistic.

Remember, though, that it is physically quite possible that the initial ratios of the samples were significantly correlated with their Rb/Sr (or other parent/daughter ratio), in which case the MODEL-3 assumptions are invalid. For a good example of such a case, see Juteau and others, 1984.

MODEL-3 is offered as an option if the program recognizes, from numbers in the axis names, that you are plotting isochron data for Rb-Sr, Sm-Nd, U-Pb (either 206/204-238/204 or 207/204-235/204), or Th-Pb. The 95% confidence-limit errors are calculated from t times the INCLUDING SCATTER errors.

MODEL-4 Yorkfits: -- A MODEL-4 Yorkfit is used only for U-Pb isotope data on a concordia diagram. This model assumes that the points scatter due to a combination of the assigned errors plus "geological" errors in the $^{207}\text{Pb}/^{206}\text{Pb}$ ratios. These "geological" errors are assumed to increase linearly from the upper concordia-intercept to the lower concordia-intercept (or vice-versa; see below). This model (see Davis, 1982, for another approach to this problem) may be appropriate for cases where a multi-episodic disturbance is suspected (in which case the closer the point to the upper intercept the greater its weight), and for cases where a significant degree of inheritance of older zircons is suspected (in which case the closer the point to the lower intercept the greater its weight). You may choose whether the lower concordia-intercept or the upper concordia-intercept is to be the age of interest.

The MODEL-4 Yorkfit is offered only for data sets with 6 points or more. The 95% confidence-limit errors are calculated by multiplying the INCLUDING SCATTER errors by the t value for $N'-2$ degrees of freedom, where N' is a number that is in general less than the actual number of points. This approach is necessary because of the way in which the MODEL-4 algorithm weights the points -- the more concordant that point, the greater its weight. In the extreme case, with 2 nearly-concordant points plus any number of much less concordant points, the algorithm will in effect pay attention only to the two most-concordant points and ignore the others. Obviously, in this case the true degrees of freedom are much less than the apparent degrees of freedom. To compensate for this effect, N' is calculated by assigning each of the two most-concordant points a "point value" of 1, and then assigning the remaining points a fractional "point value" based on their MODEL-4 weights; the less their MODEL-4 weight, the smaller a fraction of a whole "point" is assigned.

The effect of this procedure is to drastically reduce the degrees of freedom assigned to many data sets, especially if 1 or 2 of the points in the set are much more concordant than the rest. So the data sets which are most appropriate for the MODEL-4 approach are those with a large number of points that are relatively evenly-spaced along a linear trend. Data sets with few points will tend to have MODEL-4 errors that are very large, due to the large (up to several tens or even hundreds) Student's- t multiplier invoked. You can tell the value of N' used by the algorithm from the printout, which refers to the NUMBER OF EQUIVALENT "POINTS".

OBTAINING ISOCHRON AGES FROM YORKFIT LINES

If your plot is an isochron plot (including $^{207}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$ and $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{204}\text{Pb}/^{206}\text{Pb}$), the computer will automatically calculate an isochron age and error from the Yorkfit results. The decay constants used are those recommended by the I.U.G.S. Subcommittee on Geochronology (Steiger and Jager, 1977).

A WORD ABOUT 3-POINT ISOCHRONS

You should be aware that the actual uncertainties of isochron ages for regression lines with only 3 or 4 data points and no apparent "geological" scatter can be significantly greater, in many cases, than that calculated by most regression algorithms, including that of ISOPLOT. The reason for this is that with only 1 or 2 degrees of freedom (3 or 4 data points), the probability of getting an M.S.W.D. of close to 1 even though some "geological" scatter exists in the population is significantly greater than zero. For such data sets, the lack of resolution of this "geological" scatter can be expected to occur in a significant number of cases, and, because the use or non-use of a very large (12.7 for N=3) Student's-t multiplier is involved, can lead to a large underestimate of the true isochron uncertainties. For this reason, you should avoid the use of 3-point isochrons or concordia chords) if possible.

RE-USING YORKFIT POINTS and PLOTTING ERROR-ENVELOPES

After the program has completed a Yorkfit, the softkeys will be defined as:

HELP			ADD POINTS	CONTINUE
ERROR ENVELOPE			DELETE POINTS	NEW PLOT

If you press CONTINUE, you will return to the SELECT PLOTTING-SYMBOL screen, and any data-points that you enter will be treated as a new batch of points for any subsequent Yorkfits or other regressions. If you want to either add or delete from the set of points that was just Yorkfit, press the appropriate softkey. If you want to plot the 95% confidence-limit error-envelope about the Yorkfit line, press the ERROR ENVELOPE softkey. You can request an error envelope by pressing CTRL E from the SELECT PLOTTING-SYMBOL and most other screens, incidentally.

SELECTING A DASHED OR SOLID YORKFIT LINE

The Yorkfit line will be drawn as a dashed line (figure 2), unless you specify a solid line by pressing the **SOLID LINE** softkey from the **SELECT PLOTTING-SYMBOL** screen. The dash pattern will change with each successive Yorkfit (up to 5) that you request for a given plot .

THE OPTIONS SCREEN

The **OPTIONS** screen (available from the **SELECT PLOTTING-SYMBOL** screen) allows you to fit a curve to data or to change the error-input format. The softkeys are labeled as follows:

NEW SYMB.-SIZE	ABS ERRORS	% ERRORS	1-SIG ERRORS	2-SIG ERRORS
	SIMPLEX	SPLINES	POLYFIT	ESCAPE

FITTING A CURVE TO DATA

Polynomial Curves: -- The **POLYFIT** option (k8) will fit a least-squares polynomial of order 1 to 4 to the last set of plotted data. You don't need to have errors assigned to the points to fit one of these curves, but if you do include errors for a polynomial fit, the program will use these errors to weight the points and to calculate an M.S.W.D. Remember that the M.S.W.D. (mean square of weighted deviates) parameter is a measure of the goodness-of-fit of the curve, and that a value close to 1 indicates that the points scatter about as much as would be predicted by their assigned errors.

Spline Curves: -- If a polynomial curve doesn't adequately describe the trend of the data, you may want to try fitting a *spline* curve (k7 from the **OPTIONS** screen). The **SPLINES** menu looks like this:

A spline curve is a collection of cubic polynomials that connect a set of X-Y points without breaks in slope.

The **AKIMA SPLINE** and **NORMAL SPLINE** options will draw slightly different types of curves. The **AKIMA SPLINE** option also constructs curves through the upper and lower Y-error limits if Y-errors are defined for the points.

But if you don't want the spline to be forced through every point, use the **SMOOTH SPLINE** option. A **SMOOTH SPLINE** is constructed through the points in a least-squares sense, and is especially useful if the data set contains many points with resolvable scatter.

Use the **SR AGES** option if you've just plotted the data-set for a global-marine Sr-isotope trend with time and you want to solve for the age and age-uncertainty corresponding to a given Sr-isotope ratio and the just-plotted global-marine data-set.

AKIMA SPLINE		NORMAL SPLINE		SMOOTH SPLINE
		SR AGES		ESCAPE

A spline curve is a collection of cubic polynomials that are joined at each data-point and pass through each data-point, without discontinuities in slope. The disadvantage of a spline curve is that it doesn't have a convenient analytical expression (since it's a collection of many different polynomials) and, because the curves are forced precisely through each point, there is no analytical expression for the error of the curve.

Normal and Akima Splines: Both the **NORMAL SPLINE** and **AKIMA SPLINE** options will construct such a spline curve for the last-plotted data-set. The **NORMAL SPLINE** (figure 7) is a classical cubic spline, without breaks in its second derivatives as well as its first derivatives. For data sets where there are rather sharp changes in slope at some points, the **NORMAL SPLINE** curve may yield undesirable oscillatory artifacts. For such data, you may want to try the **AKIMA SPLINE** (Akima, 1970), which permits much sharper bends of the curve at each point. If your data has Y-errors associated with it, the **AKIMA SPLINE** option (figure 8) will also construct curves for both the upper and lower Y-error-limits to the data.

Smoothed Splines: If you're dealing with a large data-set and you believe that these points scatter for some reason about the most-reas-

onable X-Y curve (perhaps due to analytical error), you may want to try the SMOOTH SPLINE option (figure 9). This routine constructs a sort of spline curve that minimizes the scatter of the points (in a least-squares sense) at each segment of the curve, instead of being forced through each point.

You'll have to specify the minimum X-interval over which the curve-segments will "pay attention" to the data, and the minimum number of points to be used for each segment. The curve is constructed as a sort of moving average, in which only a quarter of the curve-segment is drawn for each least-squares fit. The larger the X-interval specified and the larger the minimum number of points for each interval, the more "smoothed" the curve will be. You'll probably have to experiment to get the parameters that are most suited to your data, so use the CRT for your preliminary trials.

You also have the option of plotting the "error-envelope" of the smoothed spline. This "error envelope" is another pair of spline curves that should enclose most of the data points defining the smoothed spline, and will pinch and swell according to the local scatter of points along the spline. *This envelope does not have rigorous statistical significance, however, and should be used mainly as a visual guide to the precision of the curve.*

Fitting a Curve to an Arbitrary Equation (Simplex Method): -- If you're willing to write a line or so of your own program code, you can fit a curve for virtually any equation to your data using a very powerful least-squares approach called the Simplex method. The Simplex method is slow and it doesn't give you any error-estimates for the parameters, but it will work for almost any equation that you can write down, and with very little mathematical or programming effort. The approach used in ISOPLOT's routine was adapted from the description (but not the program code) given in Caceci and Cachieris (1984).

To enter your equation into the program, do the following steps (don't bother to enter your data first):

- 1) Bring up the **OPTIONS** screen from the **SELECT PLOTTING-SYMBOL** menu; make sure that the ISOPLOT - AUXILIARY PROGRAMS disk is in one of the disk drives, and select **SIMPLEX (k6)** from the **OPTIONS** menu.
- 2) When the **SIMPLEX** code has been loaded into memory and the **SIMPLEX** instructions appear on the screen, type in **EDIT Eqn.** The screen will display lines of program code, with the center line looking something like this:

24510 Eqn:RETURN Param(1)+Param(2)/X+Param(3)*X^2

You must rewrite this line so that it contains your equation. The `Param()` variables are the parameters that the Simplex procedure will solve for -- up to 8. Indicate all occurrences of the X-variable in your equation with `X`. For example, the equation in the sample line above is for the equation

$$Y = C_1 + C_2/X + C_3/X^2,$$

where the Simplex procedure will solve for the best values of the equation-constants C_1 , C_2 , and C_3 . You can use more than one program line for your equation, if necessary.

- 3) When you've typed in your equation correctly, enter it by pressing the `ENTER` key. If you get an error message, you'll have to figure out what you did wrong, and try again. When you've got it right (or if you give up trying), re-start `ISOPLOT` by pressing the `RUN` key.
- 4) Enter your data into `ISOPLOT` in the usual way, and re-invoke the Simplex procedure from the `OPTIONS` menu again. This time, though, both the Simplex procedure and your equation will already be in memory, so all you need to do is press `CONTINUE` after the Simplex instructions appear on the screen, and then respond to the query,

ENTER THE NUMBER OF PARAMETERS (<8) TO BE SOLVED FOR:

- 4) Enter the number of parameters in your equation. Now respond to the query,

ENTER ESTIMATED VALUES FOR THE 5 PARAMETERS
(try all 1's if you have no idea at all)

If you have some idea of what the best values for the n parameters in your equation might be, enter these n values, separated by commas. The order of your entry must correspond to the parameter-numbering sequence used in your equation definition.

- 5) The Simplex procedure will start solving for the best values of the equation parameters. The results for each iteration, as well as the standard deviation of the points about the trial curve for each iteration. The process is not rapid, compared to most least-squares solutions, but it almost certainly will converge, given enough time. It is common for the procedure to make very little headway in the first dozen

iterations or so, so be patient. If the procedure converges precisely to stable values, it will terminate and give you the results. There is no limit on the number of iterations that it will do, however, so if you get tired of waiting, press the **ACCEPT** softkey (k0) to accept the current values. Often, even though the process has not converged to the last decimal place for each parameter, it will be very close to the best values (or at least to acceptable values), so don't be discouraged if you need to do this. When the procedure does converge, it usually takes at least 50 or even 200-300 iterations, (typically several minutes or more) so do wait a bit before pressing **ACCEPT**.

- 6) When the procedure is terminated, either from convergence or by the **ACCEPT** command, it will display the values of the equation-parameters and draw the curve (figure 10). If you wish to fit more data, or try new starting-values, you can do so without going through steps 1 through 3.

CHANGING THE ERROR FORMAT

The **% ERRORS**, **1-SIG ERRORS**, and **2-SIG ERRORS** options allow you to change the assumed form of your error input. The default error-input is at the 2-sigma level and in percent. Press the appropriate softkeys to change the assumed error-input, then press **ESCAPE** when you're done. You can also do this from the starting screen by pressing **CTRL E**.

CHANGING THE SIZE OF ALPHANUMERIC PLOTTING-SYMBOLS

You can change the size of alphanumeric plotting-symbols (key-board characters such as +, X, *, or A, 5, H) by pressing k0 from the **OPTIONS** screen. The relative size that you specify for these plotting-symbols will remain valid until you either change the size again, or begin a new plot.

CREATING CONCORDIA PLOTS

If your plot is a conventional concordia plot, with $^{206}\text{Pb}/^{238}\text{U}$ plotted against $^{207}\text{Pb}/^{235}\text{U}$, you'll find a few differences from the normal X-Y plotting routines. To select a concordia plot, press C from the starting screen; the top line of the screen will change to read **CONCORDIA PLOTTER**.

Instead of asking directly for the X- and Y limits when you're setting up the plot, the program will now ask you to:

ENTER AGE LIMITS AS: [MIN. AGE,] MAX. AGE

(or press CONTINUE to define in terms of X and Y limits)

If you enter 1 value only, the minimum age on the plot will be zero, and the value you enter will be the maximum age (in Ma). If you enter 2 values, the plot will show ages from about the first value (or slightly less) to about the second value (or slightly more).

If you want to define the plot limits in terms of the actual X- and Y-values, though, just press CONTINUE in response to the above query; the program will then ask you for those specific limits.

The concordia curve can be drawn with 2 kinds of ticks and tick labels: ticks as small circles labeled horizontally to the left of the tick, and ticks with short dashes normal to the concordia curve, with labels above and collinear with the ticks. You can select which style you want from the starting display with softkey k3 (labeled either DASH CTICK or CIRCLE CTICK).

When you request a Yorkfit through data on a Concordia plot, the program will automatically calculate the intercepts of the Yorkfit line with the concordia curve, and the uncertainties of those intercepts. These uncertainties are calculated using the algorithm developed by Ludwig (1980), and are printed out in two forms: symmetrical but approximate uncertainties, and the true, asymmetric uncertainties. You can choose which to use.

FORCING A YORKFIT LINE THROUGH A SPECIFIED AGE

You can force a Yorkfit through a specified age on the concordia curve from either the SELECT PLOTTING-SYMBOL or ADD POINTS screens. One of the prompts on the screen will be:

press CTRL F to force Yorkfit line through a point on concordia

After pressing CTRL F, you will be asked what age (in Ma) to force the next Yorkfit through, and what uncertainty to assign to this forcing age. The uncertainty value is optional -- if you enter only one value, the uncertainty in the forcing age will be assumed to be zero. If you do enter an uncertainty value, the program will calculate the Yorkfit line and concordia intercepts three times, forcing the line through not only the forcing age but also the forcing age plus and minus its assigned uncertainty. The propagated uncertainties in the unforced intercept arising from this procedure will be included in the final age-uncertainties of the unforced intercept.

The uncertainty in the forcing age is assumed to be symmetric; that is, you cannot enter a forcing age with uncertainties of +100 Ma and -50 Ma.

After any Yorkfit, the program will calculate the concordia intercepts of the Yorkfit line and its associated uncertainties, using the algorithm of Ludwig (1980). These intercepts will be labeled on the lower-right corner of the plot (optional for CRT plots), with the labels for each successive solution for a given plot stacked on top of the previous labels.

CONSTRUCTING A CONTINUOUS-DIFFUSION CURVE FOR COUPLED LOSS OF RADIOGENIC-Pb AND ^{238}U RADIOACTIVE DAUGHTERS

Some systems -- notably low-temperature uranium ores and low-temperature uraninite (pitchblende) and coffinite -- continuously leak both radiogenic-Pb and one or more of the several radioactive daughters of uranium. I have noted that for many such systems, the ratio of the leakage of Pb to the radioactive daughters must have been roughly constant over the age of the material, so that a particular type of continuous-diffusion curve can be useful in evaluating the age of the material (Ludwig, Simmons, and Webster, 1984).

To construct such a curve, press CTRL C from the SELECT PLOTTING-SYMBOL screen. You will then be asked to specify the age of the system and the ratio of diffusion constants for Rn compared to Pb, divided by 10^{10} . Radon may not, in fact, have been the actual daughter that was leaking out of the system (Ra seems to be the dominant wanderer in many cases), but the shape of the curve is the same for any daughter. Try diffusion-constant ratios in the range of 0.05 to 5 to get a feeling for the shape of the curves. For any specific set of data points, you'll have to find the best-fit curve by a trial-and-error process of varying the assumed age of the system and the assumed diffusion-constant ratio. There is no provision for estimating errors.

OBTAINING GROWTH CURVES FOR Pb-ISOTOPE PLOTS

If your plot is either for $^{207}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$ or for $^{208}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$, after drawing the plotbox and labels the program will ask you:

DO YOU WANT TO INCLUDE A SINGLE-STAGE GROWTH-CURVE IN THE PLOT?

press k0 for a Stacey-Kramers growth-curve,
k1 for some other growth-curve,

press k9 to decline growth curve.

If you press k0, the program will draw a single-stage Pb-isotope growth-curve using the constants suggested by Stacey and Kramers (1975). If you press k1, the program will ask you to define your own single-stage growth curve, requesting: (1) the starting age of the system, (2) the initial isotope ratios, (3) the μ^1 of the source, and, for $^{208}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$ plots, (4) the Th/U of the source. The screen will look like:

SINGLE-STAGE Pb-ISOTOPE GROWTH-CURVE

SELECT PARAMETER TO CHANGE WITH KNOB OR UP/DOWN ARROWS,
ENTER NEW VALUE, PRESS EXECUTE WHEN DONE.

(press k0 to restore Stacey-Kramers Parameters)

	(Stacey-Kramers values)
206/204 at start of growth	11.152
208/204 at start of growth	31.230
Mu (present-day 238/204) of source	--->9.74
Present-day 232/238 or source	3.78
Time before present (Ma) at start of growth	3700
(add an asterisk to specify a starting-age on the current growth-curve)	

Use the KNOB or the arrow-keys to move the cursor to the value you want to change, type in the value and press ENTER. You needn't change values which are already acceptable. To restore the values in the form to the standard Stacey-Kramers values (Stacey and Kramers, 1975), press k0.

If you want to start a new growth curve at some particular age on the growth curve defined by the parameters first appearing on the screen, you can have the program calculate the appropriate 206/204 and 207/204 or 208/204 ratios for this age by entering the age with an asterisk in the "Time...at start of growth" cell. For example, if you

¹Mu is defined as the $^{238}\text{U}/^{204}\text{Pb}$ of the system, normalized for U-decay to the present day.

wanted to construct a growth curve that started from the Stacey-Kramers curve at 2700 Ma and evolved with a μ of 12, you would:

- 1) press **k0** to restore the Stacey-Kramers values (if the initial values on the screen were not the Stacey-Kramers values);
- 2) type in **2700*** in the "Time..." cell and press **ENTER**. The 206/204 and 207/204 or 208/204 values immediately change to the values defined by a 2700 Ma age on the Stacey-Kramers growth curve;
- 3) enter a value of 12 in the " μ " cell and press **EXECUTE**.

Once you select a growth curve the display will become:

Press **k4** to suppress growth-curve ticks,

Press **k2** to suppress only the labels of the growth-curve ticks,

Press **k0** to draw the growth curve complete with labeled age-ticks

Because the plot may become too "busy" if the growth-curve age-ticks and age-tick labels are included, you can select how much labeling you want to include, as indicated above.

For Pb-isotope plots, the **SELECT PLOTTING-SYMBOL** screen will also allow you to add additional growth-curves (press **CTRL G**), and also to plot one or more Pb-Pb isochrons using the parameters of the last-plotted growth-curve (press **CTRL T**).

PLOTTING RARE-EARTH ELEMENT DATA

To plot rare-earth element data in the usual way (Y-semilog with the X-axis being the labeled atomic numbers of the REE), press **Z** from the starting screen. You must then specify the Y-axis label (for example, SAMPLE/CHONDRITE), and Y-range. You must type in your REE data, as no datafile support is offered.

To enter your data, when requested type in each point on the graph for a given sample as the REE element-symbol, then the Y-value, separated by a comma. For example, **La,1234 EU,.148 sm,542** are all legal responses. You will probably want to connect the points with a line after plotting (**CTRL ^** from the **SELECT PLOTTING-SYMBOL** screen). An example of an REE plot is shown in figure 5.

CALCULATING WEIGHTED AVERAGES OF A SINGLE VARIABLE

You can use **ISOPLOT** to calculate weighted averages of a single variable by pressing **A** from the starting screen. The program will then ask for data and errors for only one variable rather than two, will use the Y-axis to show that variable, and use the X-axis to show the "set number" of the data points.

You can use data from a **VISICALC** file as input just as for other plotting modes, except that you will be asked to specify two and only two columns (the values and their errors) of data.

If there is no excess scatter of the data being averaged (that is, the M.S.W.D. is near 1), the weighted averages algorithm simply weights each point by its inverse variance and calculates the uncertainty in the average value from the assigned uncertainties for each point. If there is excess scatter (M.S.W.D.>1), the average is calculated by assuming that the data scatter due to a combination of their assigned errors plus an unknown, "external" variance that has a normal (Gaussian) distribution¹. In these cases, the most probable value of the "external sigma" arising from the external variance is also calculated.

PLOTTING DATA AS A HISTOGRAM

You can plot the data for a single variable in histogram form (figure 6) by pressing **H** from the starting screen. You will then be asked to :

ENTER CELL-WIDTH, X-MIN., X-MAX.

Enter 3 values, separated by commas: (1) the desired width of the histogram cells (in general, choose a value such that the data occupy between 5 and 20 cells), (2) the lowest X-value to appear on the histogram, and (3) the highest X-value to appear on the histogram (X is the parameter for which you want the histogram).

If you type in your data from the keyboard, enter only one value per entry -- there are no X-values, and any Y-errors are irrelevant.

¹The algorithm for this approach was developed by Brent Troutman of the U.S. Geological Survey.

To get data from a datafile, press the GET DATAFILE softkey from the starting display (after having specified a histogram plot with the H key), select which datafile, and specify the single column which contains the values for which you want the histogram. You can, if you want, use data that is already in memory from a just-completed X-Y plot or weighted averages; just remember that the Y-values of the datafile will be used in this case.

Before constructing the histogram, you will be asked to choose a fill-pattern for the histogram cells. The options are: No Fill, Solid Fill, NorthEast Diagonals, NorthWest Diagonals, and Cross-Hatch.

After the histogram is constructed, you can plot a new data-set on the same histogram by selecting the NEW POINTS option. The next set of points that you enter will then be plotted on the same histogram, with a different fill-pattern if you so specify.

If you want to see how closely the histogram data match a normal or lognormal distribution, press the softkey labeled **NORMAL CURVE** or **LOGNORMAL CURVE**. The program will then construct the appropriate curve for the data.

UTILITY FUNCTIONS FOR ISOTOPIC DATA

Several utility functions are included in ISOPLOT for the user of radiogenic-isotope data. Functions, available from the starting screen, are:

- 1) Calculation of radiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ ages:-- Press 1. Enter either the radiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ ratio (1 value) or the $^{206}\text{Pb}/^{204}\text{Pb}$ and $^{207}\text{Pb}/^{204}\text{Pb}$ ratios uncorrected for common-Pb (2 values). In the latter case, the common-Pb ratios are assumed to lie on the Stacey-Kramers growth-curve for the calculated age.
- 2) Calculation of model-Pb age and Mu : -- Press 2. Enter the $^{206}\text{Pb}/^{204}\text{Pb}$ and $^{207}\text{Pb}/^{204}\text{Pb}$ ratios of the isotopic composition of interest. The program will calculate a model age and Mu^1 assuming a Stacey-Kramers single-stage growth-curve.

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

- 3) **Calculation of model-Nd age:** -- Press 3. Select whether you want the model age calculated assuming a chondritic source with constant Sm/Nd or a depleted source. Enter the $^{147}\text{Sm}/^{144}\text{Nd}$ and $^{143}\text{Nd}/^{144}\text{Nd}$ ratios of the sample. You can adjust the parameters of both the chondritic-source model and the depleted-source model to correspond to both your geologic assumptions and laboratory normalization.
- 4) **Calculation of model-Sr age:** -- Press 4. Similar to the calculation of a model-Nd age, except that the depleted-source option is not offered.

Calculation of Ages from Marine-Carbonate Sr-Isotope Ratios: -- An additional utility provided by ISOPLOT VERSION 2 calculates ages from $^{87}\text{Sr}/^{86}\text{Sr}$ ratios of marine carbonates (phosphates, sulfates...) using a standard trend of global-marine $^{87}\text{Sr}/^{86}\text{Sr}$ with age. To access this utility, you must first plot such a global-marine trend, either in the form of $^{87}\text{Sr}/^{86}\text{Sr}$ versus age or as some simple function of $^{87}\text{Sr}/^{86}\text{Sr}$ (such as delta-values relative to modern seawater) versus age. The data-set for this trend is of your own choosing.

For convenience, the data sets of Koepnick and others (1986), Hess and others (1986), DePaolo (1986), and Capo and DePaolo (1986) have been put on the ISOPLOT -- AUXILIARY disk and stored as files named **MOBIL_SR**, **HESS_SR**, and **UCLA_SR**, respectively. The latter file contains combined data from DePaolo (1986), Capo and DePaolo (1986), and Richter and DePaolo, 1987 (diffusion-corrected data). The Sr-isotope data are given in two ways in these files -- as measured $^{87}\text{Sr}/^{86}\text{Sr}$, and as Delta- ^{87}Sr , where the latter is the difference in parts per thousand between the sample $^{87}\text{Sr}/^{86}\text{Sr}$ and modern-seawater $^{87}\text{Sr}/^{86}\text{Sr}$.

When you've plotted the global-marine trend of your choice, select the **OPTIONS** menu (available from the **SELECT PLOTTING-SYMBOL** screen) and specify the **SPLINES** option. From the **SPLINES** menu, select the **SR AGES** option. You will be asked to specify a Perfect Fit or a Smoothed Curve to the global-marine trend data.

If you specify a Perfect Fit, the routine will fit an Akima-method spline to the data, where the curve is forced through each data-point on the trend. This is appropriate for relatively sparse, very-high precision data-sets such as that of DePaolo (1986). For large global-marine-trend data-sets with resolvable non-analytical scatter, such as those of Koepnick and others (1985) or Hess and others (1986), however, you should specify a Smoothed Curve. The attributes of both of these curve-types are briefly described in the section on **FITTING A**

CURVE TO DATA.

ISOPLOT will ask you to enter the $^{87}\text{Sr}/^{86}\text{Sr}$ value of the unknown-age sample and the uncertainty in that value. Again, you can use other ways of expressing the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio such as delta-values, so long as the form of the ratio is the same as that used for the global-marine trend. The procedure is as follows:

- 1) All ages (intercepts) along the global-marine trend (spline curve) that have the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of your unknown are determined. If there is only one such age, it is used as the best age-estimate. If there are several such ages, their average is used.
- 2) The intercepts of the upper and lower limits (from your assigned error) on the sample $^{87}\text{Sr}/^{86}\text{Sr}$ ratio with the global-marine trend are located. The differences between the resulting maximum and minimum ages and the best age-estimate are used to calculate variances in the positive and negative age directions, and assigned to a sample-error variance.
- 3) The intercepts of the sample Delta- ^{87}Sr with the spline curve constructed through all of the upper limits of the calibration curve are determined, then the intercepts of the spline curve constructed through all of the lower limits of the calibration curve. In the case of a normal spline or Akima spline calibration curve (that is, a curve passing through each of the calibration points), the upper and lower limits are taken to be spline curves constructed through the upper and lower error-limits of the points. In the case of a smooth spline, the limits reflect the 2-sigma statistical error about the curve. The differences between the maximum and minimum ages from these intercepts and the best age estimate are used to calculate variances in the positive and negative age-directions, and assigned to a global-marine-trend variance.
- 4) The upper and lower errors on the best age-estimate are determined by taking the square roots of the sums of the variances from sample error and from global-marine-trend error. Because the upper and lower errors are determined separately, they need not be symmetric about the best age estimate.

UTILITIES FOR DISK-FILE MANAGEMENT

INITIALIZING DISKS

Before you can use a new disk to store datafiles (or programs), you'll have to initialize (format) the disk. You can do this from either the VISICALC or BASIC operating system, but it may be more convenient to take advantage of the program's built-in initializing function. Just press D from the starting screen, then follow the instructions. You can initialize either one or two disks at a time. Remember that the initialization process will wipe out all information that might already be present on the disk, so be careful.

If you intend to use the initialized disks for **VISICALC** files, remember the name that you chose for the disk (even better, write the name on the disk label). This is the "volume label" or "volume name" that VISICALC needs to know in order to access files on the disk.

COPYING FILES OR ENTIRE DISKS

You can copy either individual files or entire disks with ISO-PLOT's file-copying utility. Press F from the starting screen, then follow the instructions. Remember that the disk you're copying files to must not be write-protected. Also remember that if you choose the disk-copy option to copy all of the files on a disk, that you will wipe out any existing files on the target disk.

PACKING THE FILES ON A DISK

The HP BASIC operating system tends to leave lots of empty areas on a disk that may be too small to hold large files, so that there is a lot of wasted space. To consolidate these fragmented empty areas into a single large area, and so be able to effectively increase the capacity of the disk, you can invoke HP's file-repacking utility from ISO-PLOT. Press K (for Krunch) from the starting screen to invoke this utility, which is reasonably self-guiding. If the utility isn't already in memory, ISOPLOT will tell you to put the **AUXILIARY** disk in one of the drives before proceeding.

DUMPING A CRT PLOT TO THE PLOTTER OR PRINTER

You can obtain a hard copy of any CRT plot by requesting that the CRT plot be dumped to either the printer or the plotter. Press CTRL P from the **SELECT PLOTTING-SYMBOL** screen to dump to the printer, CTRL D to dump to the plotter. The printer-dump will only work if the printer is one of the types that can accept direct graphics-dumps, such as the HP-2225 (ThinkJet) and HP-82906 printers. Plotter dumps will always use a plot-size of 8 and pen-number 1.

REFERENCES

- Akima, Hiroshi, 1970, A new method of interpolation and smooth curve fitting based on local procedures: J. Assoc. Computing Mach., v. 17, p. 589-602.
- Brooks, Christopher, Hart, S.R., and Wendt, Imold, 1972, Realistic use of two-error regression treatments as applied to rubidium-strontium data: Rev. Geophys. Space Phys., v. 10, p. 551-577.
- Caceci, M.S., and Cacheris, W.P., Fitting curves to data: the Simplex algorithm is the answer: Byte, May 1984, p. 340-362.
- Capo, R.C., and DePaolo, D.J., 1986, Pleistocene Sr isotope stratigraphy and paleoceanography: Geol. Soc. America Abstracts with Programs 1986, v. 18, p. 557.
- Davis, D.W., 1982, Optimum linear regression and error estimation applied to U-Pb data: Canadian Journal of Earth Sciences, v. 19, p. 2141-2149.
- DePaolo, D.J., 1986, Detailed record of the Neogene Sr-isotopic evolution of seawater from DSDP Site 590B: Geology, v. 14, p. 103-106.
- Hess, Jennifer, Bender, M.L., and Schilling, J.-G., 1986, Evolution of the ratio of Strontium-87 to Strontium-86 from Cretaceous to present: Science, v. 231, p. 979-984.
- Juteau, Martine, Michard, Annie, Zimmerman, Jean-Louis, and Albareda, Francis, 1984, Isotopic heterogeneities in the granitic intrusion of Monte Capanne (Elba island, Italy) and dating concepts: Jour. Petrology, v. 25 p. 532-545.
- Koepnick, R.B., Burke, W.H., Denison, R.E., Hetherington, E.A., Nelson, H.F., Otto, J.B., and Waite, L.E., 1985, Construction of the seawater $^{87}\text{Sr}/^{86}\text{Sr}$ curve for the Cenozoic and Cretaceous: supporting data: Chemical Geology, v. 58, p. 55-81.
- Ludwig, K.R., 1980, Calculation of uncertainties of U-Pb isotope data: Earth Planetary Science Letters, v. 46, p. 212-220.
- , 1983, Plotting and regression programs for isotope geochemists, for use with HP-86/87 microcomputers: U.S. Geological Survey Open-File Report 83-849; 89 p.
- , 1985, ISOPLOT200, A plotting and regression program for isotope geochemists, for use with HP Series 200 computers: U.S.

Geol. Survey Open-File Report 85-513: 105 p.

- , 1985, PBDAT200, a computer program for processing raw Pb-U-Th isotope data: U.S. Geological Survey Open-File Report 85-547; 90 p.
- , Simmons, K.R., and Webster, J.D., 1983, U-Pb isotope systematics and apparent ages of uranium ores, Ambrosia Lake and Smith Lake districts, Grants Mineral Belt, New Mexico: Economic Geology, v. 79, p. 322-337.
- McIntyre, G.A., Brooks, Christopher, Compston, William, and Turek, Andrew, 1966, The statistical assessment of Rb-Sr isochrons: Jour. Geophys. Research, v. 71, p. 5459-5468.
- Richter, F.M., and DePaolo, D.J., 1987, Numerical models for diagenesis and the Neogene Sr-isotopic evolution of seawater from DSDP Site 590B: Earth Planetary Science Letters, v. 83, p. 27-38.
- Stacey, J.S., and Kramers, J.D., 1975, Approximation of terrestrial lead isotope evolution by a two-stage model: Earth Planetary Science Letters, v. 26, p. 207-221.
- Steiger, R.H., and Jager, Emilie, 1977, Subcommission Geochronology: Convention on the use of decay constants in geo- and cosmochemistry: Earth Planetary Science Letters, v. 36, p. 359-362.
- Titterton, D.M., and Halliday, A.N., 1979, On the fitting of parallel isochrons and the method of maximum likelihood: Chemical Geology, v. 26, p. 183-195.
- York, Derek, 1969, Least-squares fitting of a straight line with correlated errors: Earth Planetary Science Letters, v. 5, p. 320-324.

FIGURE CAPTIONS

- Figure 1: Example of an X-Y plot where the plotting-symbols are, from left to right, open and filled error-boxes, error-cross, open and filled error ellipses, asterisk, open 20-sided polygon, open 3-sided polygon with vertex at 90° , filled 3-sided polygon with vertex at 270° , open six-sided polygon with vertex at 90° , filled 5-sided star (=polygon with -5 sides) with vertex at 90° , open 20-sided star (=polygon with -20 sides). Curve is best-fit third-degree polynomial to these points, plot-size is 7.
- Figure 2: Example of a Concordia plot with 4 points shown as error ellipses and the Yorkfit line (dashed) from these points. Also shown are the 95% confidence-limit error-envelope and labeled concordia-intercepts for the Yorkfit line.
- Figure 3: Example of a stacked plot using the usual axes for a common-Pb isotope plot. Curves are Stacey-Kramers growth curves, with points on the curve labeled in Ma.
- Figure 4: Example of a semi-log X-Y plot, with polynomial curves fit to two data sets.
- Figure 5: Example of a Rare-Earth Element plot and REE pattern.
- Figure 6: Example of a histogram plot, with lognormal curve superimposed on the histogram.
- Figure 7: Example of a "normal" spline curve, without errors (data of Capo and DePaolo, 1986).
- Figure 8: Example of an "Akima-method" spline curve, with errors (data of Capo and DePaolo, 1986).
- Figure 9: Example of a smoothed spline curve, with errors (data of Koepnick and others, 1985).
- Figure 10: Example of a best-fit curve (to points shown in figure) using the Simplex method.
- Figure 11: Plot making use of a variety of ISOPLOT's features. The arrows are a combination of solid error-boxes and solid triangles (polygons); the inset was positioned using the "NONSTANDARD" option of the PLOT-SIZE query; the small-delta symbol is obtained with the CTRL-D character; the curve is an Akima-type spline fit to data plotted with the "spacebar" character (no markings used).

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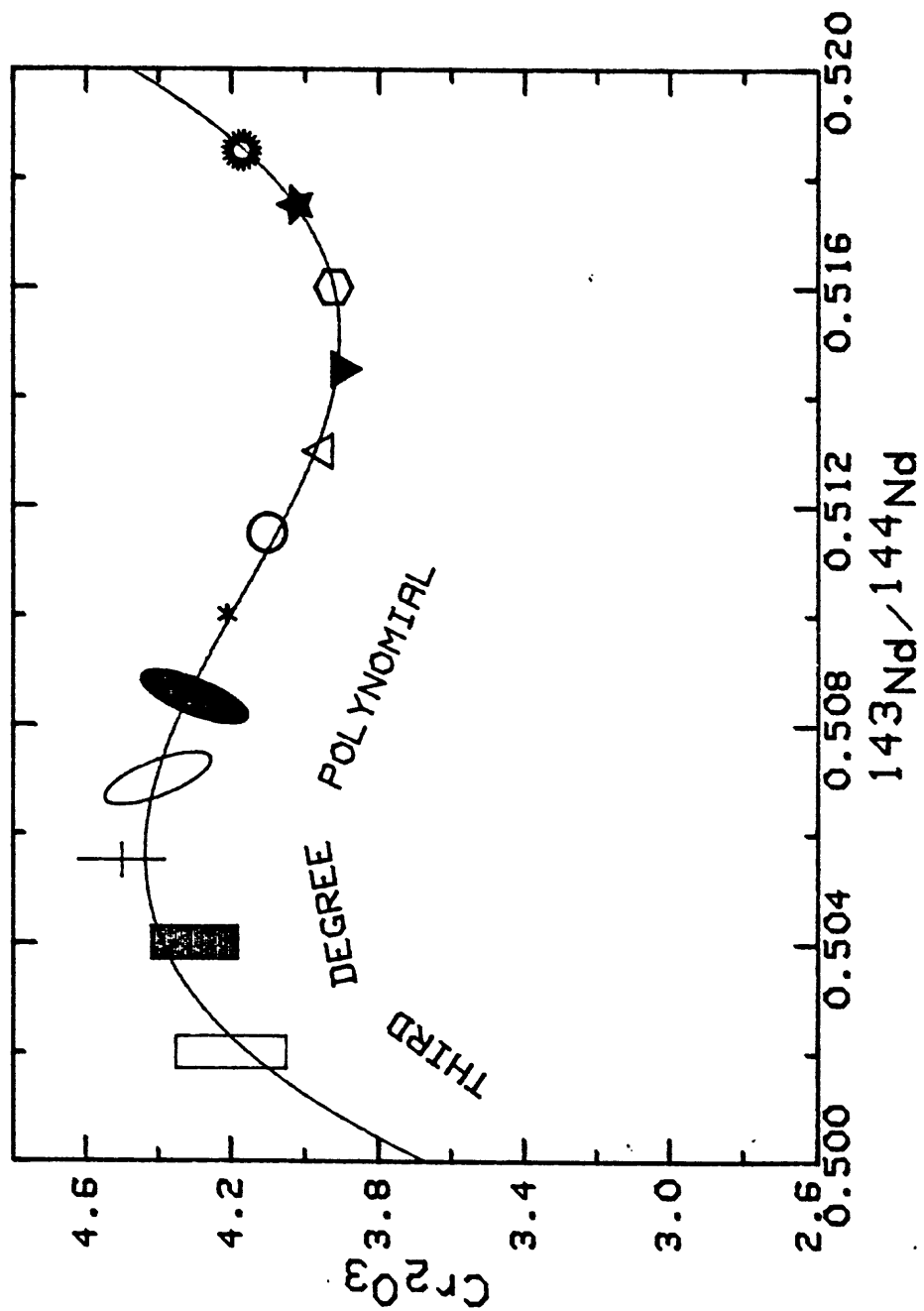


Figure 1

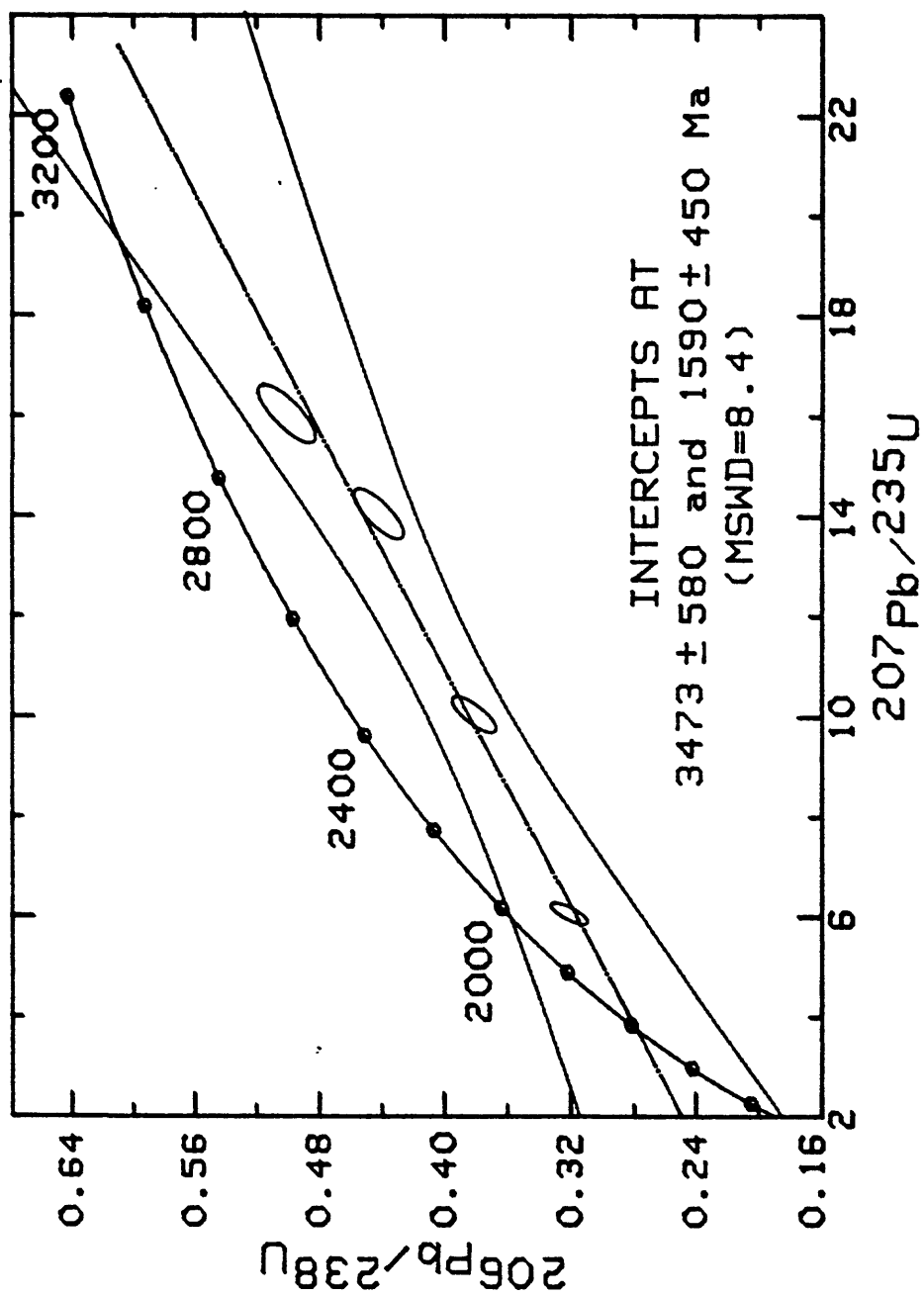


Figure 2

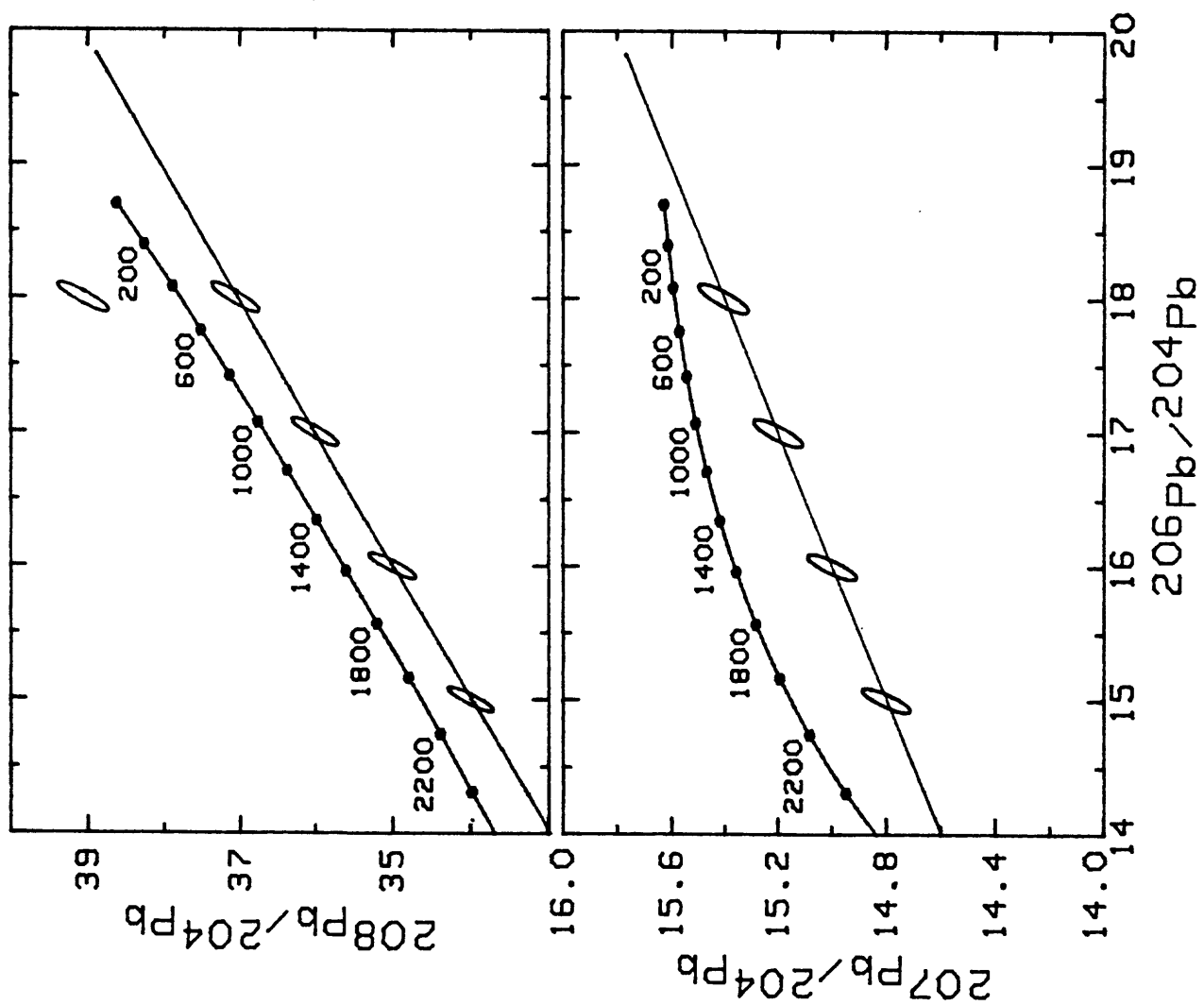


Figure 3

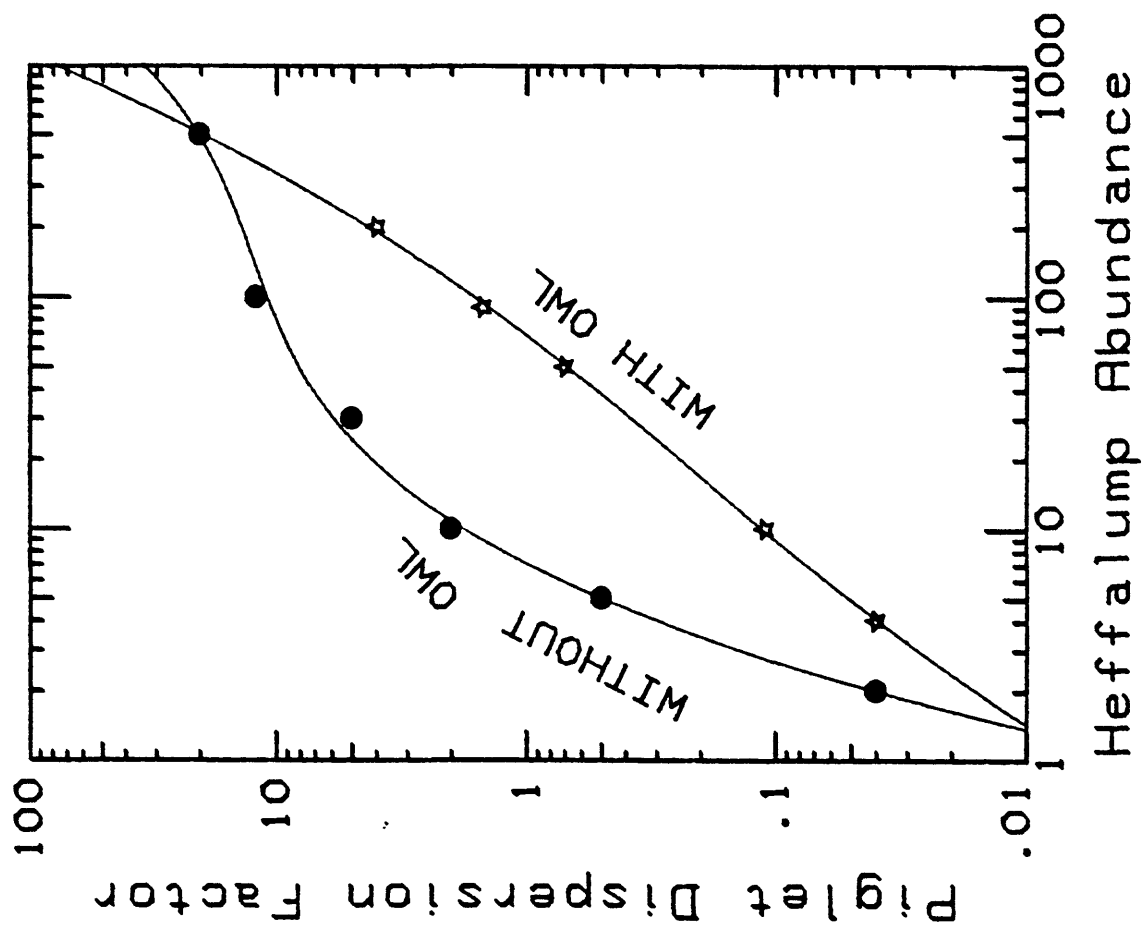


Figure 4

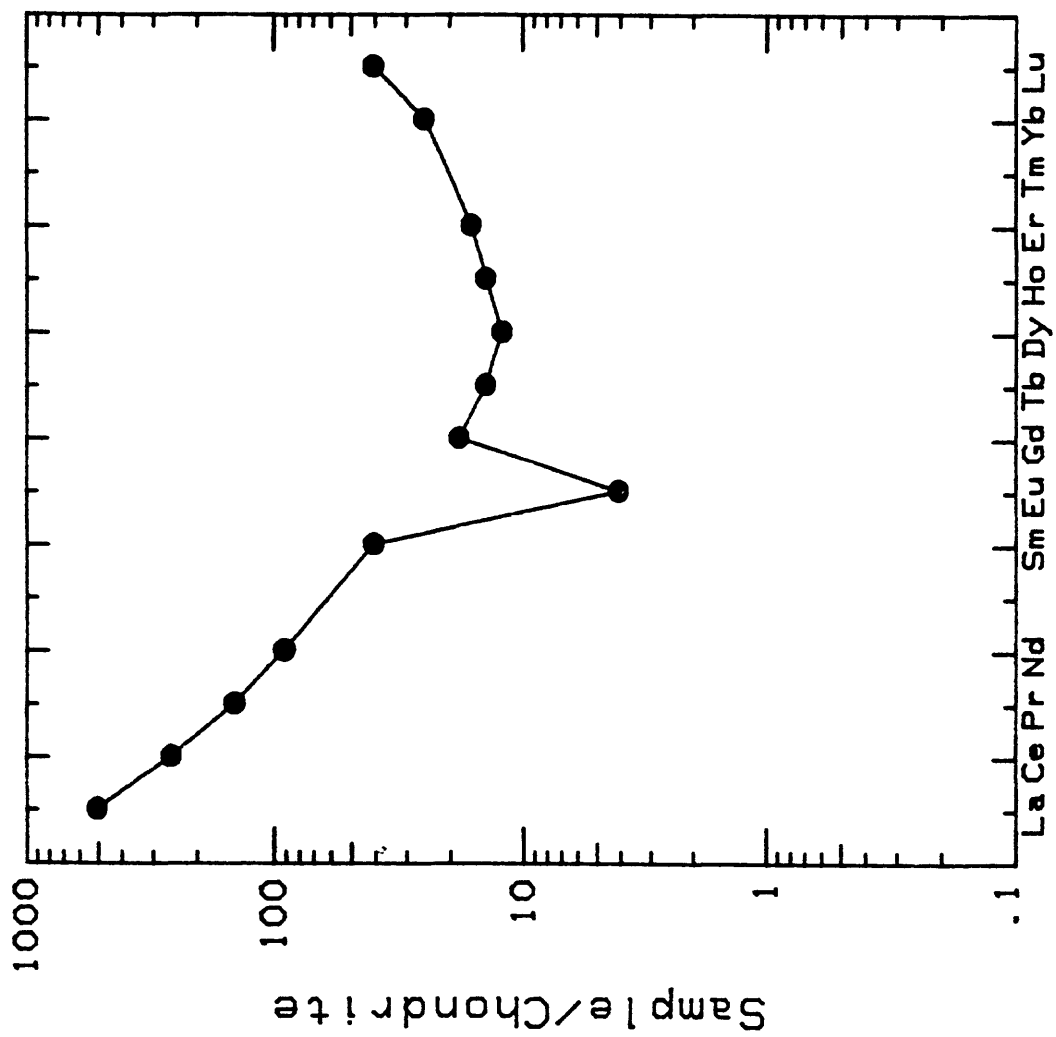


Figure 5

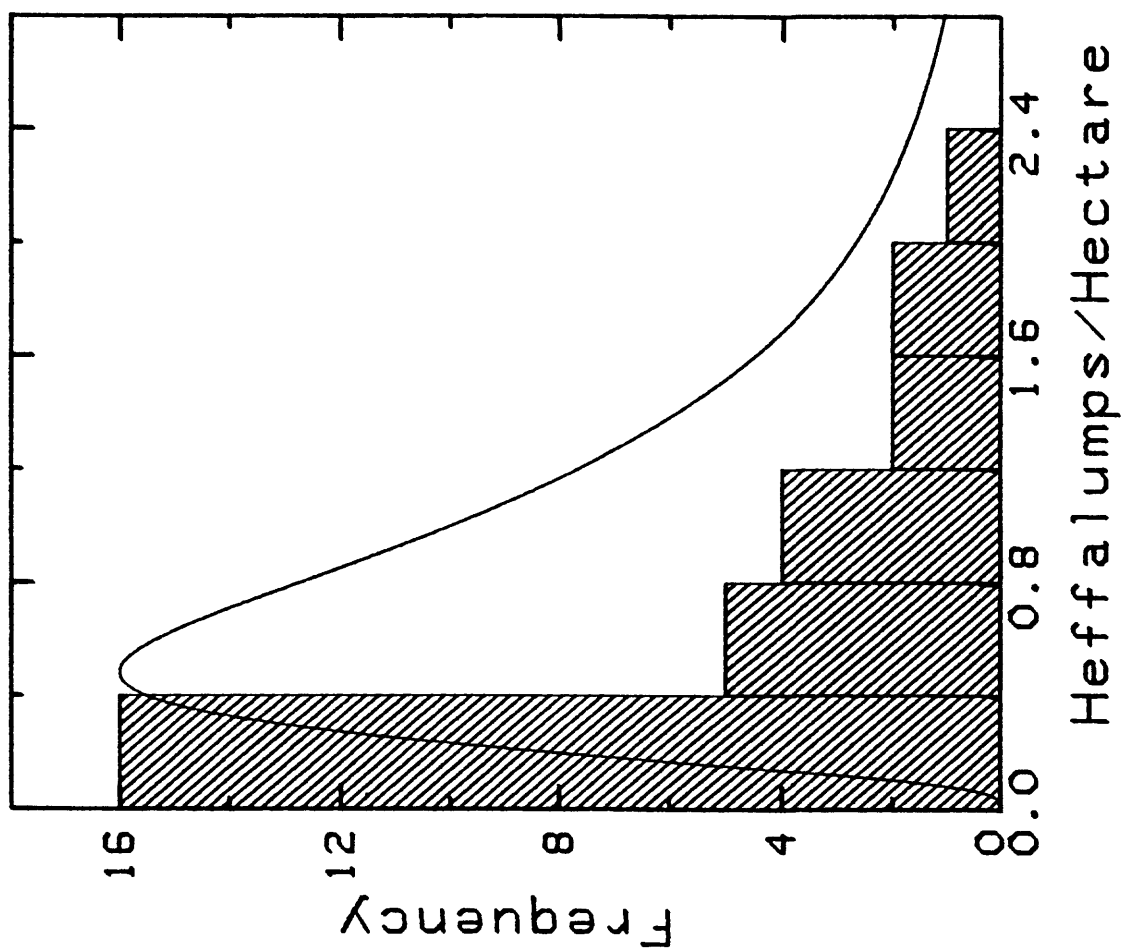


Figure 6

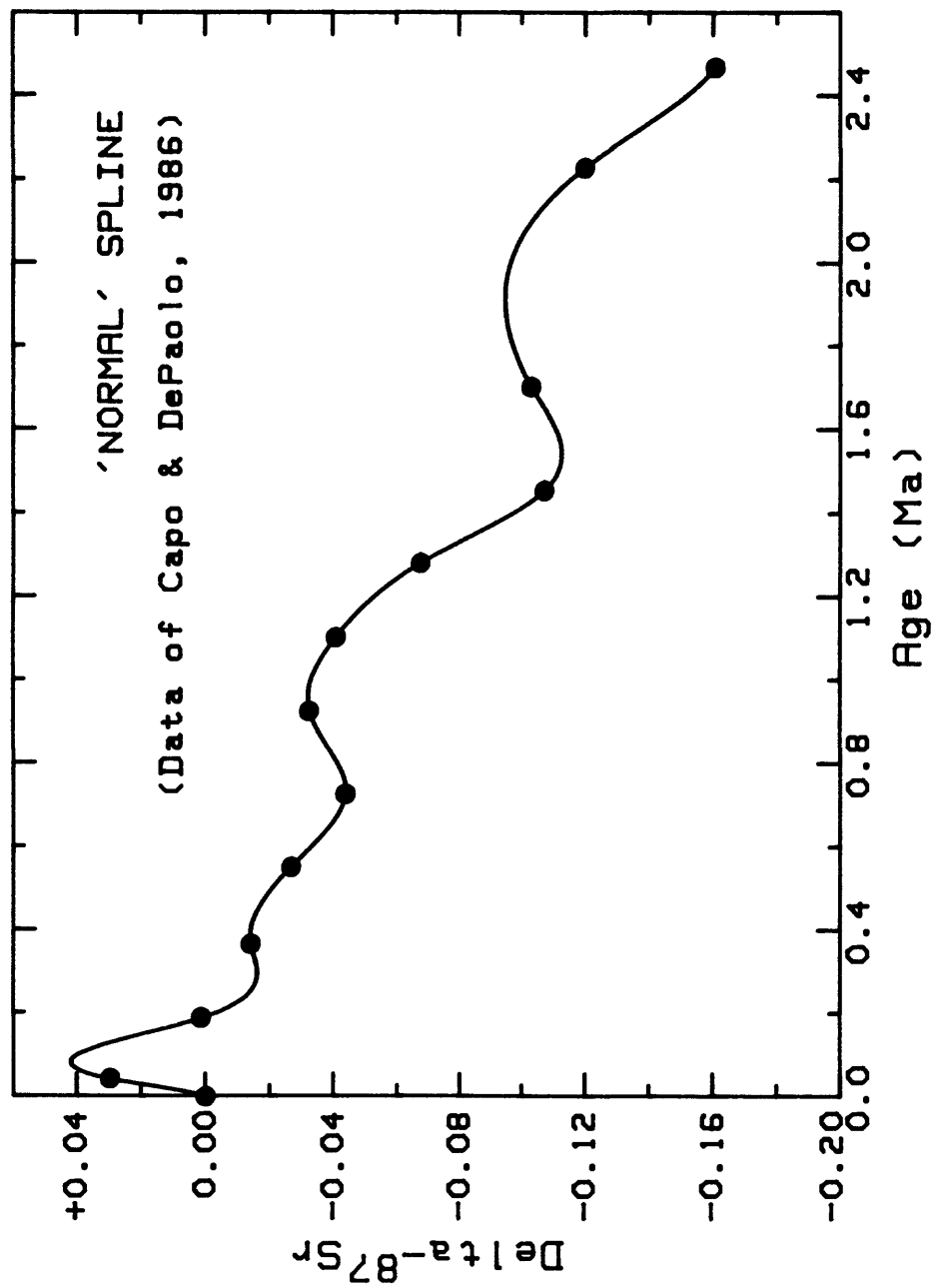


figure 7

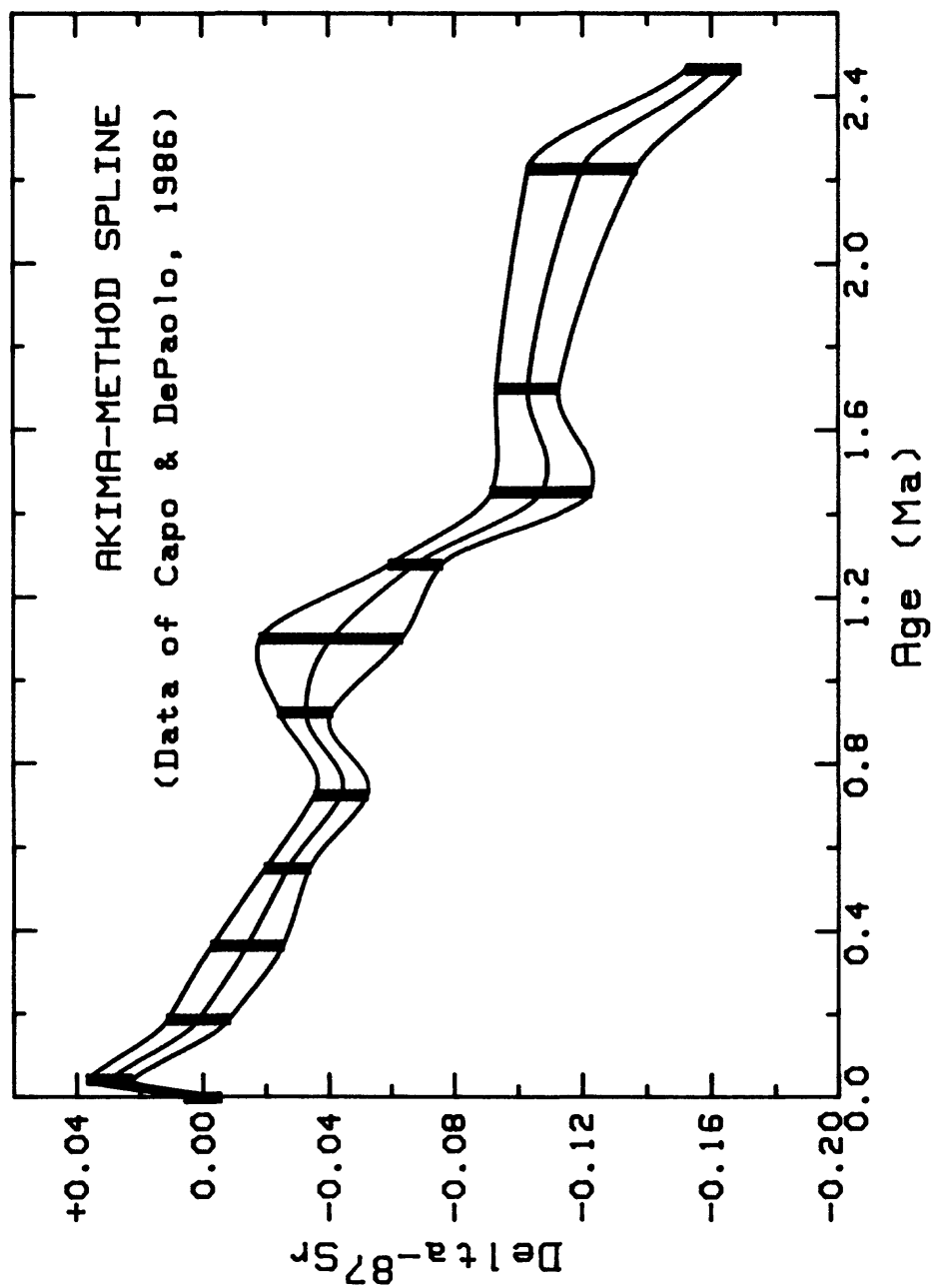


figure 8

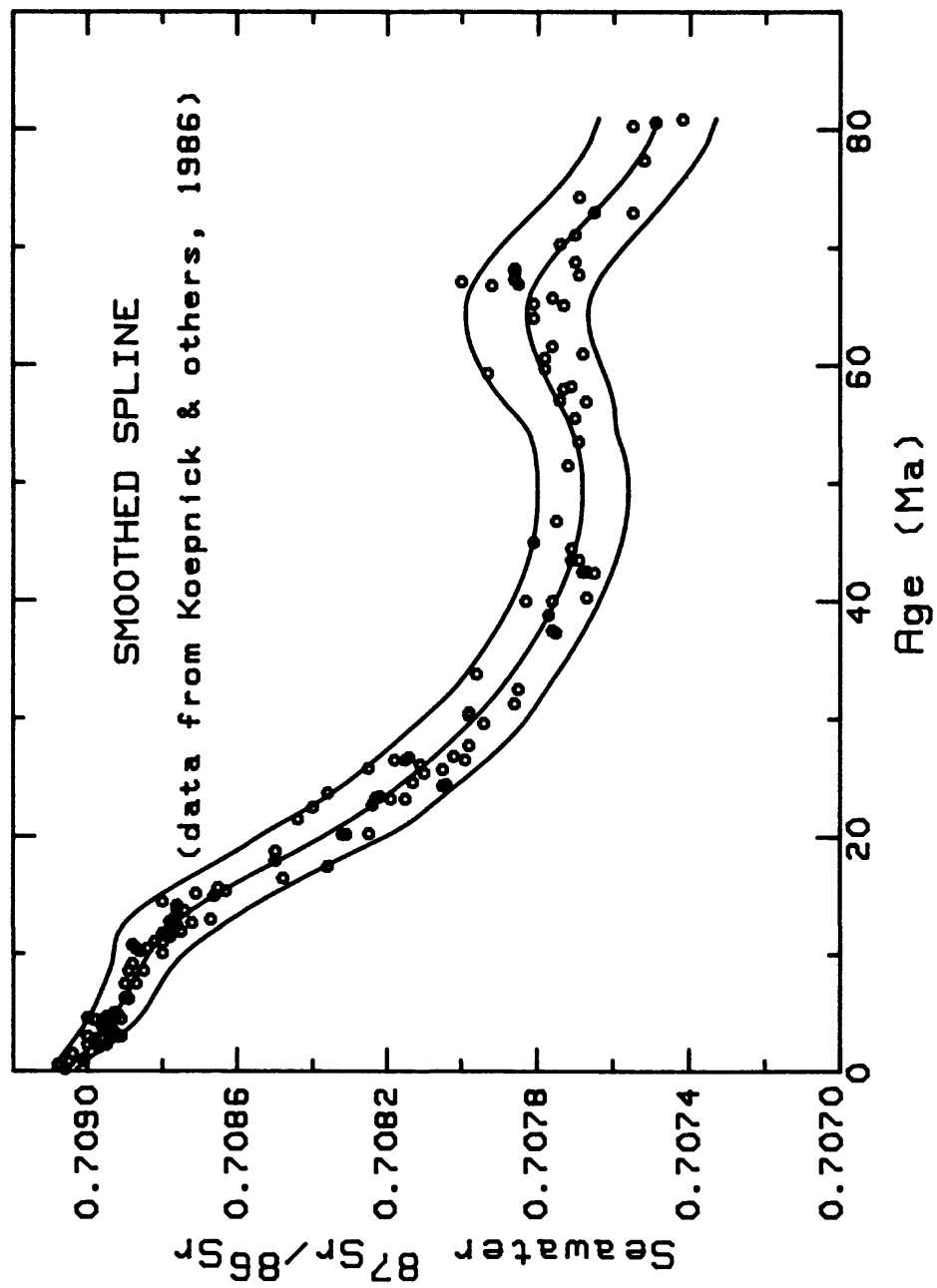


figure 9

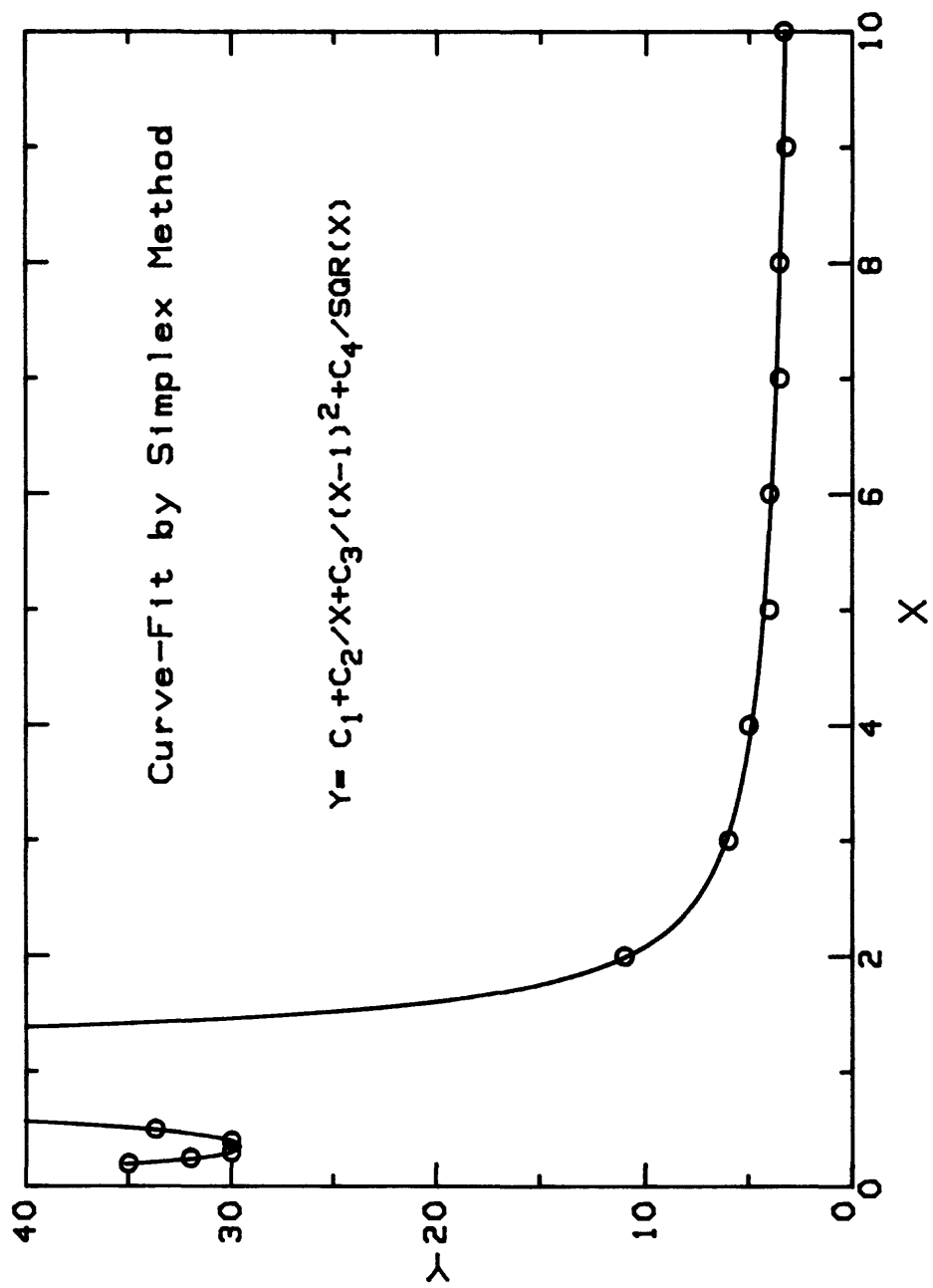


figure 10