

DEPARTMENT OF THE INTERIOR

U. S. GEOLOGICAL SURVEY

Plotting Programs for Rare Earth Elements,
Spider Diagrams, and Ternary Diagrams

by

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Open-File Report 88-9

This report is preliminary and has not been reviewed for conformity with U.S. Geological Survey editorial standards (and stratigraphic nomenclature).

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INTRODUCTION

REE.BAS--Rare earth plotting program
SPIDER.BAS--Spider diagram plotting program
TERNARY.BAS--Ternary diagram plotting program

These programs were written in BASIC and HP-GL for an IBM AT computer with an HP 7475A plotter. The screen display is a monochrome monitor with an EGA graphics card.

The communication parameters for all three programs are set as follows:

Baud rate = 9600
No parity
8 data bits
1 stop bit

You must set the DIP switches on the back of the plotter to agree with these settings, or you must alter the program to match the settings of your plotter. The OPEN statement (line number 80 in REE.BAS and SPIDER.BAS and line number 3220 in TERNARY.BAS) is OPEN "COM1:9600,N,8,,RS,CS65535,DS,CD" AS #1 in each of the programs.

Screen graphics, that is, the display of the graph on the screen, are written specifically for the kind of monitor and graphics card used. In this case, with a monochrome monitor and EGA card, I have set SCREEN 10. You may need to use SCREEN 1 (Medium resolution graphics mode [320x200]--use with Color/Graphics Monitor Adapter only) or SCREEN 2 (high resolution graphics mode [640x200]--use with Color/Graphics Monitor Adapter only). The SCREEN statement is in line number 11105 in REE.BAS and 11050 in SPIDER.BAS. No screen graphics are used in TERNARY.BAS.

Included on the disk are versions of the program that will run on a WANG PC with the HP 7475A plotter using a monochrome monitor and graphics card. The main differences between the two versions of the program are screen graphics, the format of an input data file, and the reading of that file.

The disk also contains sample input files for each of the programs--Ree.dat, Spider.dat, and Ternary.dat. Although the files do not contain realistic values they will give the user an example of the input file format.

This documentation is included on the disk and can be printed out from DOS by using the Print Screen function in combination with the TYPE command.

REE.BAS PROGRAM OVERVIEW

RUNNING REE.BAS

The program is a combination of menu-driven selections and screen prompts.

***** HOME MENU *****

- 1) Input Data/Begin New Plot
- 2) Draw Axis
- 3) View Plot on Screen
- 4) Plot Data (after step 2)
- 5) Enter Title, Y-axis Label, and Symbol Labels
- 6) Plot Title, Y-Axis label, and Symbol Labels

- 7) Enter or change Y-axis Label
- 8) Plot Y-axis Label
- 9) Enter or change Title
- 10) Plot Title
- 11) Enter or change Symbol Labels
- 12) Plot Symbol Labels
- 13) Normalize Data

- 14) Exit Program

The Home Menu is divided into 3 sections for ease of use. You can do everything you need to do using the first 6 items on the menu. Numbers 7-13 are included to speed things up in certain circumstances. For example, menu item #5 asks you for all three pieces of information, so if you wanted to change only one of the three it would be more efficient to use menu items 7-13 to do so. That is, if all of your plots had the same symbol labels and Y-axis label, but the title changed each time, you would want to enter all three pieces of information once, and then with each subsequent plot use menu item #9 to enter just the title. (Then use #6 to plot all three at once.) Another example--after data input the program loops directly to the normalization routine. However, if you wanted to try a different normalization routine on numbers you had already entered and normalized, you could use menu item #13 to do so. In this way you would not have to go through the "Input Data" portion to get to the normalization routine.

Menu item #14 exits the program entirely. Do not use it to begin another plot. Select menu item #1 to begin a new plot.

DATA INPUT

The program will accept data from an ASCII file (no more than 100 samples per file) or from the keyboard. Data entered from the keyboard, however, will not be saved on disk. When entering data, either from the keyboard or from a data file, you must enter 0 if you do not have a value for a particular element.

When data is read from a file you select the samples you wish to plot by entering the index number of the sample to be used for each plot group. These index numbers are listed, along with the sample names, in the sample list optionally provided by the program. They are printed out when the list of sample names is generated, so it is a good idea to print out this list at least once. By assigning new index numbers to be plotted you can plot various combinations of samples from the same data file.

DATA INPUT (continued)

Values are remembered until you enter new ones from the keyboard or read them in from a new file. Therefore, you can do multiple plots with the same data, varying things such as normalization routine, without entering the data each time.

If you use data input from a file, and want to make a number of plots using various combinations of the samples in the file, you need to read the file only once. Read the file the first time, then when you want to make the subsequent plots from that same data file select "Input Data" again from the Home Menu and answer "Y" to the question, "Do you want to use the same file as last time?". When a different file is desired simply respond "N" and you will be prompted to enter a new file name.

INPUT FILE FORMAT

An ASCII file must be in a particular format to be read by the program. The first line should be the total number of samples in the file. Subsequent lines contain data for up to 100 samples. Data for each sample consists of 2 lines. The first line contains the sample name or number, up to 10 characters. The second line contains values for the 15 rare earth elements, separated by spaces or commas, in the following order:

La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu

If you do not have a value for a particular element, you must enter a zero--do not skip that field.

***** S A M P L E F I L E *****

3

SAMPLE 1

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

SAMPLE 2

10 20 30 40 50 60 70 80 90 100 110 120 130 140 150

SAMPLE 3

100 200 300 400 500 600 700 0 900 1000 1100 1200 1300 1400 1500

PLOT GROUPS AND SYMBOLS

REE.BAS will plot up to 6 samples per plot. You may use any combination of the six plotting symbols (Cross, Triangle, Square, Diamond, Inverted Triangle, X), but it will not use more than one color.

AXES, LEGEND, AND TITLE

The Y-axis is somewhat flexible. You may choose starting and ending values of .1, 1, 10, 100, 1000 and no others. You may choose any combination of starting and ending values from the list--for instance you could go from .1 to 100 or 1 to 1000 but you could not go from 5 to 250. Since it is a log scale, it is helpful to have some idea what the range of values will be after normalization. Viewing the plot on the screen will help you decide appropriate starting and ending values.

The spacing of elements on the X-axis can be equidistant (in the order of increasing atomic number) or based on ionic radius. The element Pm is not included when plotting by ionic radius, and therefore the value zero should be entered for that element if you plan to use ionic radius spacing.

A legend can be printed on the right hand side of the plot. Symbol labels (usually sample numbers) can be entered from the keyboard or read from the file and must be no longer than ten characters. The plot title and Y-axis label are entered by the user.

VIEWING PLOT ON SCREEN

The plot is displayed on the screen without the plot title and symbol legend, and with equidistant spacing on the X-axis, even if ionic radius spacing has been selected. The Y-axis range is .1 to 1000.

NORMALIZATION ROUTINES

Four normalization routines (Haskin Chondrite, Haskin Shale, Masuda Chondrite, Anders and Ebihara) are provided, as well as the opportunity to enter your own values or to not normalize at all. The type of normalization routine used is printed at the bottom of the plot.

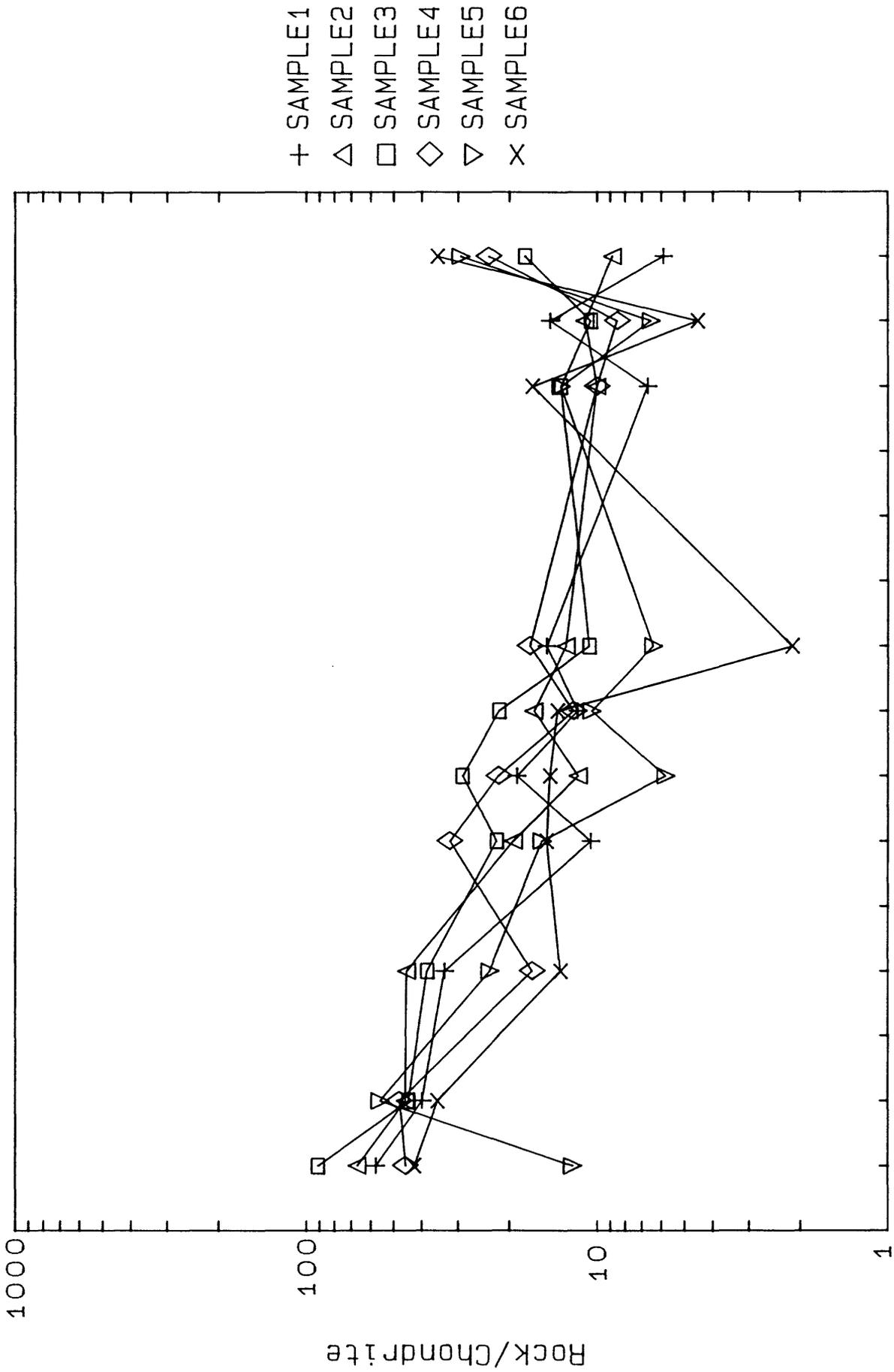
** NORMALIZATION VALUES **

	Haskin chondrite	Haskin Shale	Masuda chondrite	Anders & Ebihara
La	0.33	32	0.378	0.309
Ce	0.88	73	0.976	0.807
Pr	0.112	7.9	0.136	0.122
Nd	0.60	33	0.716	0.599
Pm	99	99	99	99
Sm	0.181	5.7	0.23	0.195
Eu	0.069	1.24	0.0866	0.0734
Gd	0.249	5.2	0.311	0.258
Tb	0.047	0.85	0.0589	0.465
Dy	0.31	99	0.39	0.321
Ho	0.07	1.04	0.0888	0.0717
Er	0.2	3.4	0.255	0.210
Tm	0.03	0.5	0.0385	0.324
Yb	0.2	3.1	0.249	0.208
Lu	0.034	0.48	0.0387	0.0321

** LIST OF VARIABLES IN REE.BAS **

VARIABLE	DEFINITION	LINE NUMBER OF FIRST OCCURENC
C(,)	Normalization values	10236
COUNT	COUNT=0 when no data has been read. After a file has been read, COUNT is incremented. This allows the user to use different samples from a file without rereading the file.	1266
CR\$	User response of readiness to begin some action	1455
D(,)	Values input from keyboard	1237
DIST1	Length of title	7010
DIST2	Length of Y-axis label	5030
DIST3	Length of normalization routine name	3003
E(,)	Result of normalization routine--D(,)/C(,)	10244
EL\$	Names of elements	77
EXTVW\$	User response to exit screen view	15620
FILE\$	Name of data file to be read	1275
I\$	User response to choose data input from keyboard or file	1091
K	Counter to increment X-position until non-zero value is found. Used while drawing lines on screen.	15311
LP\$	User response for using same data file as last time	1272
MN	Index number of Home Menu choice	360
N	Index number of data set to create (also used as counter in FOR NEXT loops)	1220
NORM\$	Names of normalization routines	10083
NT	Index number of which normalization routine to use	10079
Q	Number of samples in data file	1286
R\$	User response to choose equidistant or ionic radius X-axis spacing	2030
SAM\$	Sample name read from file	1410
SL\$	User response for listing of samples names in file	1440
SYM\$	Plotting symbols	1080
SYMLBL\$	Label for symbols. Assigned from SAM\$(Z()).	1492
T\$	Title of plot	6020
U\$	User response for more data input from keyboard	1241
V(,)	Input values read from file. Assigned to D(,) when plot groups have been chosen.	1420
V\$	Y-axis label	4040
X	X-position of X-axis labels	2415
X1	X-position of points when plotted on screen	15000
X2	X-position of <u>next</u> point when drawing lines on screen	15315
XPT	X-position of X-tic and X-position of point to plot	2224
Y1	Y-position of points when drawing lines on screen	15320
Y2	Y-position of <u>next</u> point when drawing lines on screen	15390
YB	Beginning Y-axis value	2040
YE	Ending Y-axis value	2050
YTIC	Counter to keep track of Y-axis tic cycles	2265
YPOS	Y-position of point to plot	3035
YPT	Y-position of Y-tic	2304
Z()	Index number of sample for a plot group	1481

RARE EARTH PLOTTING TEST



Haskin chondrite values (1968)

SPIDER.BAS PROGRAM OVERVIEW

RUNNING SPIDER.BAS

The program is a combination of menu-driven selections and screen prompts.

***** HOME MENU *****

- 1) CHOOSE TYPE OF SPIDERGRAM/Begin New Plot
- 2) Input Data/Begin New Plot
- 3) Draw Axis
- 4) View Plot on Screen
- 5) Plot Data (after step 3)
- 6) Enter Title and Symbol Labels
- 7) Plot Title and Symbol Labels

- 8) Enter or change Title
- 9) Plot Title
- 10) Enter or change Symbol Labels
- 11) Plot Symbol Labels

- 12) Exit Program

The crucial menu choice in this program is #1--CHOOSE TYPE OF SPIDERGRAM. You must select the type of spider diagram before you enter data the first time and before you draw axes. If you do not select a type of diagram the program will not run at all. This is because each diagram has the elements in a different order and uses different normalization values. Once you tell it what type of diagram to draw it will reorder and normalize the values based on that choice. If you want to do several of the same type of diagram you do not have to select it each time, but if you change you must remember to designate a new type of diagram.

The Home Menu is divided into 3 sections for ease of use. You can do everything you need to do using the first 7 items on the menu. Numbers 8-11 are included to speed things up in certain circumstances. For example, menu item #6 asks you for both title and symbol labels, so if you wanted to change only the title it would be more efficient to use menu item #8 to do so. So, if all of your plots had the same symbol labels, but the title changed each time, you would want to enter both pieces of information once, using menu item #6, and then with each subsequent plot use menu item #8 to enter just the title. (Then use #7 to plot both at once.)

Menu item #12 exits the program entirely. Do not use it to begin another plot. Simply select menu item #1 or #2 to begin a new plot.

TYPES OF SPIDER DIAGRAMS AND NORMALIZATION ROUTINES

The program will plot the following types of spider diagrams:

<u>TYPE</u>	<u>ELEMENTS IN ORDER PLOTTED</u>
1. General Spider Diagram	Cs, K, Rb, Ba, Th, Ta, Nb, Ce, P, Zr, Hf, Sm, Ti, Y, Yb, Eu, Sr, Zn, Sc, Mg, Co, Cr
2. Pearce--MORB normalized	Sr, K, Rb, Ba, Th, Ta, Nb, Ce, P, Zr, Hf, Sm, Ti, Y, Yb
3. Pearce--ORG normalized	K, Rb, Ba, Th, Ta, Nb, Ce, Hf, Zr, Sm, Y, Yb
4. Wood--Mantle normalized	Cs, Rb, Ba, Th, U, K, Ta, Nb, La, Ce, Sr, Nd, P, Hf, Zr, Sm, Ti, Tb, Y
5. Thompson--Chondrite normalized	Ba, Rb, Th, K, Nb, Ta, La, Ce, Sr, Nd, P, Sm, Zr, Hf, Ti, Tb, Y, Tm, Yb

**** NORMALIZATION VALUES ****

	General	Pearce MORB	Pearce ORG	Wood	Thompson
Cs	1.6	--	--	0.019	--
K ₂ O	1.27	0.15	0.4	0.03	0.015
Rb	27	2	4	0.86	0.35
Ba	485	20	50	7.56	6.9
Th	2.3	0.2	0.8	0.096	0.042
Ta	0.3	0.18	0.7	0.043	0.02
Nb	4	3.5	10	0.62	0.35
Ce	28	10	35	1.9	0.865
P ₂ O ₅	0.309	0.12	--	0.021	0.011
Zr	135	90	340	11	6.84
Hf	3	2.4	9	0.35	0.2
Sm	4.1	3.3	9	0.385	0.203
TiO ₂	0.54	1.5	--	0.255	0.103
Y	20	30	70	4.87	2
Yb	1.7	3.4	8	--	0.22
Eu	1.14	--	--	--	--
Sr	577	120	--	23	11.8
Zn	71	--	--	--	--
Sc	12.8	--	--	--	--
MgO	2.35	--	--	--	--
Co	14.6	--	--	--	--
Cr	15	--	--	--	--
U	--	--	--	0.27	--
La	--	--	--	0.71	0.328
Nd	--	--	--	1.29	--
Tb	--	--	--	0.099	0.052
Tm	--	--	--	--	0.034

You can enter your own values only on type 1--General Spider Diagram.

PLOT GROUPS AND SYMBOLS

SPIDER.BAS will plot up to 6 samples per plot. You may use any combination of the six plotting symbols (Cross, Triangle, Square, Diamond, Inverted Triangle, X), but it will not plot in more than one color.

DATA INPUT

The program will accept data from an ASCII file (no more than 100 samples per file) or from the keyboard. Data entered from the keyboard, however, will not be saved on disk. There are a total of 27 elements used in the 5 types of plots. In order to allow you to change types without entering the data again, the data entry from keyboard routine prompts you for all 27 elements in the same order as required for an ASCII input file (see page 10). The order is always the same, and does not change with the type of plot. Therefore, it is necessary to watch the prompt--IT WILL NOT NECESSARILY PROMPT YOU IN THE ORDER IN WHICH THE ELEMENTS ARE PLOTTED. Simply enter 0 if you have no value for a particular element. A data file must also contain values for all 27 elements.

When data is read from a file, select the samples you wish to plot by entering the index number of the sample to be used for each plot group. These index numbers are listed, along with the sample names, in the sample list optionally provided by the program. They are printed out when the list of sample names is generated, so it is a good idea to print out this list at least once. By assigning new index numbers to be plotted you can plot various combinations of samples from the same data file.

If you use data input from a file, and want to make a number of plots using various combinations of the samples in the file, you need to read the file only once. Read the file the first time, then when you want to make the second and subsequent plots from that same data file select Input Data again from the Home Menu and answer "Y" to the question, "Do you want to use the same file as last time?". When a different file is desired simply respond "N" and you will be prompted to enter a new file name.

The program will remember numbers entered either from disk or keyboard until you select "Input Data" from the Home Menu again. Therefore, if you want to use the same data in a different type of spider diagram you could select CHOOSE TYPE OF SPIDERGRAM and proceed with the plot without entering the data again. However, whenever you wish to change the data in any manner, (i.e. different samples entirely, or same samples in different plot group combinations) you must input data again.

AXES, LEGEND, AND TITLE

The Y-axis is somewhat flexible. You may choose starting and ending values of .01, .1, 1, 10, 100, 1000 and no others. You may choose any combination of starting and ending values from the list--for instance you could go from .1 to 100 or 1 to 1000 but you could not go from 5 to 250. It is a log scale and it is helpful to have some idea what the range of values will be after normalization. Viewing the plot on the screen will help you decide appropriate starting and ending values.

A legend can be printed on the right hand side of the plot. Symbol labels (usually sample numbers) can be entered from the keyboard or read from the file and must be no longer than ten characters.

The program determines and prints the Y-axis label, and the title of the plot is entered by the user.

VIEWING PLOT ON THE SCREEN

The plot is displayed on the screen without the plot title and symbol legend. The Y-axis range is .01 to 1000.

INPUT FILE FORMAT

An ASCII file must be in a particular format to be read by the program. The first line should be the total number of samples in the file. Subsequent lines contain data for up to 100 samples. Data for each sample consists of 2 lines. The first line contains the sample name or number, up to 10 characters. The second line contains values for ALL 27 POSSIBLE ELEMENTS separated by spaces or commas. Entering values for all elements allows the user to change types of spider diagrams without inputing data again. The elements must be in the following order:

Cs,K,Rb,Ba,Th,Ta,Nb,Ce,P,Zr,Hf,Sm,Ti,Y,Yb,Eu,Sr,Zn,Sc,Mg,Co,Cr,U,La,Nd,Tb,Tm

VALUES FOR K, P, Ti, AND Mg SHOULD BE IN WEIGHT PERCENT OXIDE ALL OTHERS IN PPM

If you do not have a value for a particular element, you must enter a zero--do not skip that field.

***** S A M P L E F I L E *****

3

SAMPLE 1

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27

SAMPLE 2

27 26 25 24 23 22 21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1

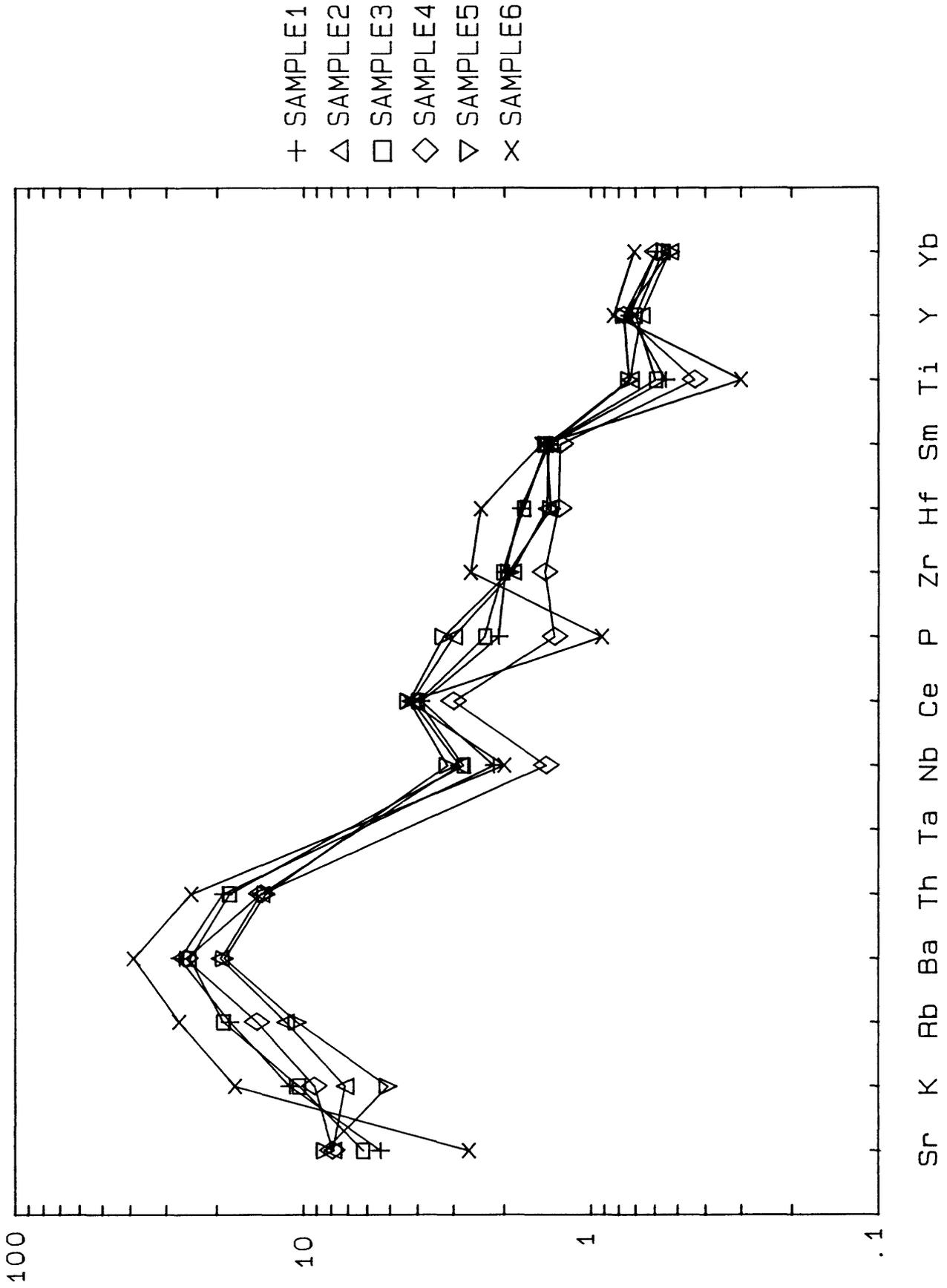
SAMPLE 3

9 5 1 3 6 8 10 11 15 16 4 6 3 21 89 34 21 25 67 87 4 21 16 17 78 4 90

** LIST OF VARIABLES IN SPIDER.BAS **

VARIABLE	DEFINITION	LINE NUMBER OF FIRST OCCURENCE
C(,)	Normalization values	1670
COUNT	COUNT=0 when no data has been read. After a file has been read, COUNT is incremented. This allows the user to use different samples from a file without rereading the file.	1532
CR\$	User response of readiness to begin some action	1035
D(,)	Values from keyboard and file after reordering	1615
DIST1	Length of title	7010
DIST3	Length of Y-axis label	2834
E(,)	Result of normalization routine--D(,)/C(,)	1695
EL\$	Names of elements <u>after</u> they have been reordered	1614
EXTVW\$	User response to exit screen view	15620
FILE\$	Name of data file to be read	1270
I\$	User response to choose data input from keyboard or file	1091
K	Counter to increment X-position until non-zero value is found. Used while drawing lines on screen.	15311
LP\$	User response for using same data file as last time	1276
MN	Index number of Home Menu choice	360
N	Index number of data set to create (also used as counter in FOR NEXT loops)	1220
NEL	Number of elements in a particular spider diagram	4065
OREL\$	List of elements in original order	77
OV\$	User response to enter own normalization values in Genral Spider Diagram	1685
PB\$	User response for getting printout of Crater Lake hypothetical andesite normalization values.	1677
Q	Number of samples in data file	1286
R	Order of elements in a particular spider diagram	1590
SAM\$	Sample name read from file	1410
SL\$	User response for listing of samples names in file	1440
SYM\$	Plotting symbols	88
SYMLBL\$	Label for symbols. Assigned from SAM\$(Z()).	1492
T(,)	Values input from keyboard	1237
T\$	Title of plot	6020
TS	Index number of type of spider diagram chosen	4046
TYPE	TYPE=1 when a spider diagram has been chosen. One must be chosen before plotting can begin.	4002
U\$	User response for more data input from keyboard	1241
V(,)	Input values read from file. Assigned to T(,) when plot groups have been choosen.	1420
X	X-position of points when plotting on screen	14300
X1	X-position of <u>originating</u> point when drawing lines on screen	15000
X2	X-position of <u>next</u> point when drawing lines on screen	15315
XD	Distance between X-tics, based on type of spider diagram, when plotted on screen.	12020
XE	End of X-axis for each spider diagram. XE=NEL+1	4080
XPT	X-position of X-tic and X-position of point to plot	2224
Y1	Y-position of points when drawing lines on screen	15310
Y2	Y-position of <u>next</u> point when drawing lines on screen	15390
YLBL\$	Label for Y-axis	2826
YB	Beginning Y-axis value	2040
YE	Ending Y-axis value	2050
YTIC	Counter to keep track of Y-axis tic cycles	2265
YPOS	Y-position of point to plot	3035
YPT	Y-position of Y-tic	2304
Z()	Index number of sample for a plot group	1481

SPIDER DIAGRAM PLOTTING TEST



TERNARY.BAS PROGRAM OVERVIEW

RUNNING TERNARY.BAS

This program plots ternary diagrams incorporating up to 100 samples, six plot groups and multiple colors. The user makes decisions in response to a series of screen prompts.

DATA INPUT

The program will accept data from an ASCII file (no more than 100 samples per file) or from the keyboard. Data entered from the keyboard, however, will not be saved on disk. All data are normalized to 100%.

INPUT FILE FORMAT

An ASCII file must be in a particular format to be read by the program, and should have NO MORE THAN 100 SAMPLES IN A FILE. Data should be in three columns--values for the lower left corner of the triangle in column 1, values for the top corner of the triangle in column 2, and values for the lower right corner of the triangle in column 3. Use the value 1111 to designate the end of a plot group, and the value 9999 the indicate the end of the file. If you want to skip a particular plot group enter 1111 as the only value for that plot group.

```
***** SAMPLE FILE *****
    50    25    25
    60    40    40
1111                                (Marks end of plot group 1)
    25    50    25
1111                                (Marks end of plot group 2)
1111                                (Skip plot group 3)
    60    25    15
    70    25    5
    90    5     5
1111                                (Marks end of plot group 4)
    20    20    60
1111                                (Marks end of plot group 5)
    60    30    10
    10    30    60
    45    45    10
    50    20    30
9999                                (Marks end of file)
```

```
*****
```

The values can be separated by spaces or commas.

PLOT TITLE AND SYMBOL LEGENDS

A title and symbol legend are optional. Both are plotted in black. Each corner of the triangle is also labelled in black.

PLOT GROUPS AND COLORS

Six plot groups are available--Cross, Triangle, Square, Diamond, Inverted Triangle, and X. Plot group 1, as well as the axes, must always be plotted in black. You can use other colors for plot groups 2 through 6 by responding "Y" to the question "Do you want to use different colors for each plot group?". After selecting the colors you will be prompted to load them in the carousel in a particular order.

** LIST OF VARIABLES FOR TERNARY.BAS **

<u>VARIABLE</u>	<u>DEFINITION</u>	<u>LINE NUMBER OF FIRST OCCURENCE</u>
ANS\$	User response to choose multiple colors	3010
CR\$	User response to indicate paper has been replaced	9006
COLR\$()	Colors for plot groups	272
FILE\$	Name of data file	1270
G\$	Indicates if a plot has been made previously	3002
I\$	User response to choose file input from disk	1091
LBL\$()	Labels for plot groups	4033
LG\$	User response to choose to include symbol legend	4025
LG1\$	User response to use same legend as last plot	4017
N	Number of data set to create during input from keyboard	1220
NAMEPLOT\$	Title of plot	4000
Q\$	User response to indicate same colors as last plot	3003
SYM\$()	Plotting symbols	281
TITLE\$()	Labels for corners of triangle	345
U\$	User response to enter data in another plot group	1247
V(, ,)	Values input from keyboard or file	1238
XPOS	X position of point	3655
YPOS	Y position of point	3650

TERNARY PLOTTING TEST

