UNITED STATES DEPARTMENT OF THE INTERIOR

GEOLOGICAL SURVEY

RAREPLOT: a computer program for plotting rare earth

element data using an IBM PC, Lotus 1-2-3,

and a Hewlett-Packard plotter

by

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Open-File Report 86-570-A

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1986

INTRODUCTION

RAREPLOT is a program for making presentation- or publication-quality plots of rare earth element (REE) data in black-and-white or color (Fig. 1). A "selected elements" option allows the user to plot axis labels only for the rare earth elements most commonly reported from instrumental neutron activation analyses.

HARDWARE REQUIREMENTS

The program was developed on an IBM PC/XT microcomputer using DOS version 3.1 and the IBM Advanced BASIC interpreter (BASICA), then compiled using the Microsoft QuickBASIC compiler to improve program execution speed. The program should run on most "PC-compatible" computers using MS-DOS version 2.0 or later. At least 256K of memory and one disk drive are required; two disk drives are preferred. Any type of display monitor and display adapter may be used. The program was developed using a Hewlett-Packard 7475A 6-pen plotter, but any multiple pen plotter using the Hewlett-Packard Graphics Language (HPGL) may be used.

FILES INCLUDED ON THE DISTRIBUTION DISKETTE

The distribution diskette contains the following files:
RAREPLOT.EXE   the RAREPLOT program.
RAREPLOT.DOC   documentation for the RAREPLOT program.
RAREDEMO.WK1   a Lotus 1-2-3 worksheet file containing a sample data set.
RAREDEMO.DIF   a sample data file, readable by RAREPLOT. It was produced by converting the RAREDEMO.WK1 file to a DIF file.

DATA ENTRY AND TRANSFORMATION

Data may be entered in any program that can convert its files to Data Interchange Format (DIF) files in "columnwise" format. The procedure for entering and transforming data using Lotus 1-2-3 is described below.

The data files must be arranged in vertical columns with a non-numeric (label) heading at the top of each column (Table 1). One blank line between the label and the start of the data is permitted but is not necessary. The program expects an entry for all 15 rare earth elements (La through Lu), so a zero or blank cell must be entered for any elements not analyzed; these will not be plotted but must be included in the data set in order for each valid data point to be plotted in the correct position on the graph. The REE data must be chondrite normalized as entered, as there is no provision in the RAREPLOT program to normalize the data. The spreadsheet must begin in cell A1 and all cells must be contiguous, i.e., there can be no totally blank columns. The data may also be taken from a larger spreadsheet by using the Lotus **/File Xtract** command to save the desired part of a larger spreadsheet. If this technique is used, be sure to specify values rather than formulas when the file is saved. The Xtracted file must then be reloaded and resaved (using the same filename) so that the resulting spreadsheet file can be properly converted to a DIF file by the Translate program.
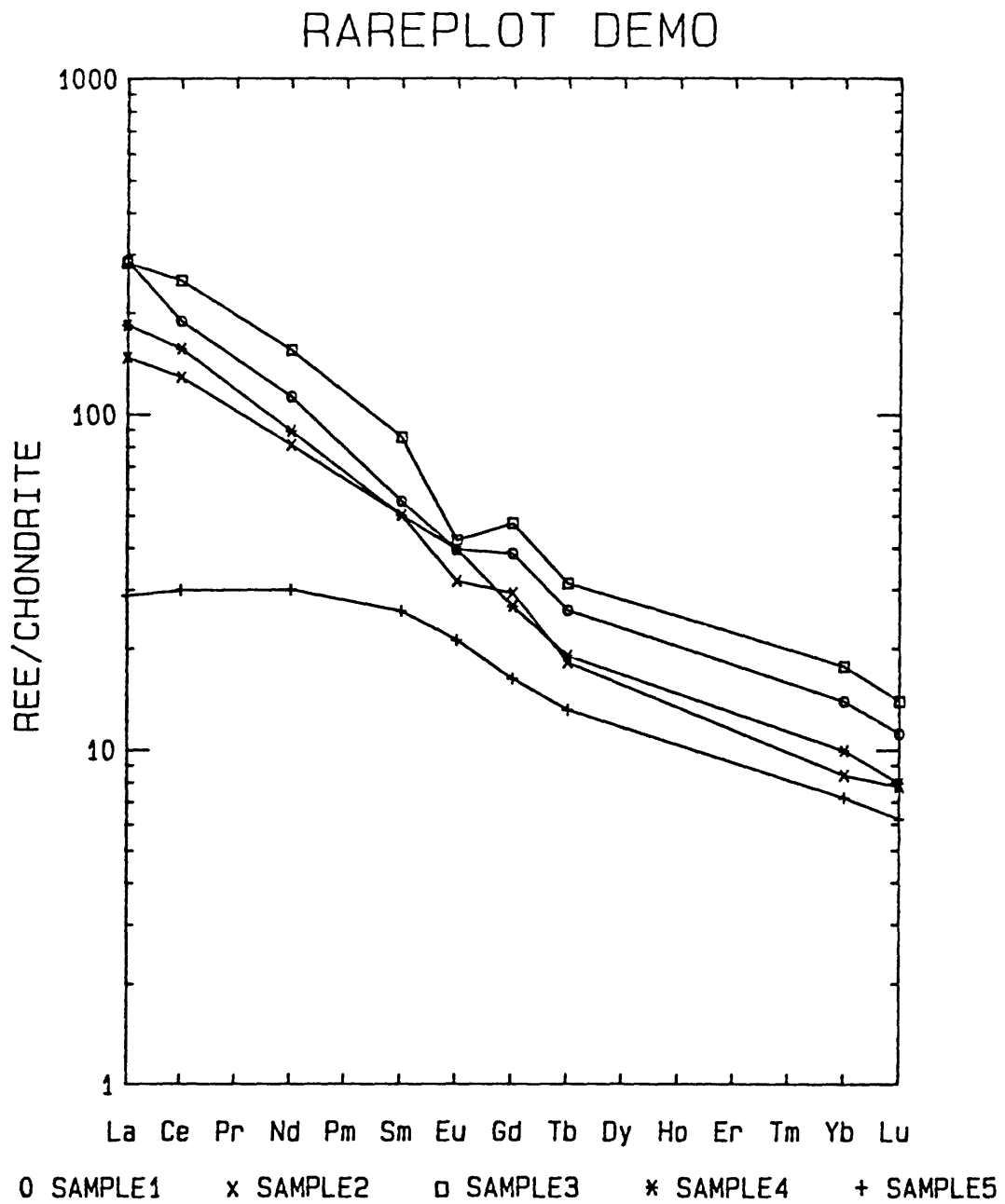
RAREPLOT DEMO

Figure 1. Sample plot generated by the RAREPLOT program.

TABLE 1. Sample Lotus 1-2-3 worksheet used for RAREPLOT data input.

SAMPLE1	SAMPLE2	SAMPLE3	SAMPLE4	SAMPLE5	SAMPLE6	SAMPLE7
286.7	147.3	283.3	183.9	28.8	22.4	153.9
188.8	128.8	250.0	156.3	29.9	20.9	160.0
0	0	0	0	0	0	0
112.7	81.1	154.9	89.2	30.0	21.2	138.1
0	0	0	0	0	0	0
55.2	50.2	85.6	50.1	25.8	15.4	92.8
39.6	31.7	42.2	39.6	21.2	15.4	70.4
38.4	29.2	47.4	26.7	16.3	12.0	65.5
26.0	18.2	31.3	19.0	13.1	7.9	40.2
0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	0	0	0	0	0	0
14.0	8.4	17.7	10.0	7.2	3.8	13.4
11.2	7.8	14.0	7.9	6.2	3.1	11.2

After exiting the spreadsheet, use the Lotus **Translate** program to translate the 1-2-3 worksheet file to a DIF file. Consult the Lotus documentation for details on this program.

USING THE DOS "MODE" COMMAND

The serial port is not automatically initialized by the RAREPLOT program, so the DOS "MODE" command must be executed prior to running RAREPLOT. The MODE command is used to set communications parameters for the serial port and takes the form

MODE COM1: 96,N,8,1,p .

In this example, serial port COM1: has been set to 9600 baud, no parity, 8 data bits, and one stop bit. The P parameter enables a continuous retry of timeout errors when the serial port (i.e., the plotter) is accessed; it is strongly recommended that this parameter be included in the MODE statement. The DOS reference manual contains a detailed explanation of the MODE command and its parameters; consult your plotter manual for a listing of the recommended communications parameter settings for the plotter. It is recommended that the MODE command be included in an AUTOEXEC.BAT file so that it is executed automatically each time the computer is started up.

RUNNING THE RAREPLOT PROGRAM

At the DOS prompt, type **RAREPLOT** and press RETURN to start the RAREPLOT program. When running the program for the first time, a setup routine titled "SYSTEM INFORMATION" is executed. You will be prompted for two pieces of information concerning your system's configuration.

The first prompt requests a drive name (and subdirectory, if desired) as a default location for data files. The default is drive B and may be selected by pressing RETURN. Any other drive specifier or directory name may be typed in place of the "B", for example "C:\PLOT\DATA", but the drive letter (C: in this example) must always be included. This tells the program where to find data files if a drive (and/or path) is not specified in response to the prompt for the name of the data file. The default may be overridden during program execution by adding a drive and path when specifying the data file name.

The second prompt is for the number corresponding to the serial port to which the plotter is connected. The choices are COM1 and COM2. To choose COM1 (the default), press RETURN. Enter a "2" and press RETURN to select COM2.

This system information is stored in a file named PLOTTER.INF and is read by the program in all subsequent runs. As long as the program is able to read this file, the setup routine will not be executed. To change the default values, delete the PLOTTER.INF file and rerun the RAREPLOT program. The setup routine will then be executed and a new PLOTTER.INF file created.

NOTE: the PLOTTER.INF file is an ASCII file containing the responses to the two prompts in the setup routine. As an alternative to deleting the PLOTTER.INF file, the parameters in this file may be easily changed using any text editor (word processor, EDLIN, etc.) capable of reading and writing ASCII files.

SELECTING PLOTTING OPTIONS

ENTER THE NAME OF THE DIF FILE CONTAINING THE DATA TO BE PLOTTED: the first
step in setting up a plot is to enter the name of the .DIF file containing the
data to be plotted, then press RETURN. If you wish to see a listing of the
DIF files on the default drive, press RETURN at the prompt. If you need to
end the program at this point, press Ctrl-Break. After this point, the only
way to terminate the program is by moving down to the last prompt on the main
menu and pressing Q to quit. If the data file is on a disk in the default
drive (as specified in the setup routine), the drive does not need to be
specified. If the file is located on a drive or subdirectory other than the
specified default, the drive and path must be specified with the file name.
The ".DIF" file extension need not be entered unless you have used a file
extension other than .DIF for the data file (this is not recommended; remember
that RAREPLOT can only read files in the DIF format). For example, if the
default drive has been set to B, then RAREDEMO, B:RAREDEMO, RAREDEMO.DIF, and
B:RAREDEMO.DIF are all acceptable entries if the file RAREDEMO.DIF is on the
diskette currently in drive B. A bar graph shows the progress of the program
as it reads the data file, then a listing of the column labels in the data
file will be displayed. Each column label will be preceeded by a number;
enter these numbers in response to the "ENTER THE NUMBER CORRESPONDING TO EACH
DATA SET TO BE PLOTTED:" prompt. The prompt for each data set is of the form
"DATA SET # n =>", where n will be 1 for the first data set, up to the number
of data columns in the file (a maximum of five data sets per run is
recommended if plot symbols are to be used, as only five plot symbols are
available). When you have selected all of the data sets to be plotted, press
RETURN at the next "DATA SET # n =>" prompt; the main menu will then be
displayed.

After the data file and data sets to be plotted have been selected, the
RAREPLOT main menu appears (Figure 2). If your computer has a color display,
the prompts will be in amber, and the user responses will be colored blue.
Each prompt turns a bright yellow when it is the "active" prompt (on a
monochrome screen, the active prompt will be brighter than the other prompts
on the menu). Pressing RETURN at any prompt causes the next prompt on the
menu to become the active prompt, as does pressing the Y or N keys in response
to prompts requiring only a yes or no response. The main menu prompts and
appropriate responses to them are discussed below:

PLOT AXES: enter Y (yes) or N (no) to select whether the axis and labels will
    be plotted prior to plotting data. Axes should always be plotted the
    first time the program is run. The "PLOT AXES:" option allows you to plot
    more than five sets of data on one pair of axes. To do this, make a plot,
    then select another set of data or another data file. Run through the
    menu as many times as necessary, responding N to the "PLOT AXES:" prompt
    after the first plot has been made. When plotting in color, you may wish
    to change the order of the pens or insert different colored pens in the
    pen carousel so that the five plot symbols will be different colors in
    subsequent plots. This way, an unlimited number of data sets may be
    plotted on a single set of axes by plotting them five sets at a time.
    Alternatively, if symbols are not plotted at each data point, you may
    specify any number of data columns for a single program run (this is most
    effective when plotting in black-and-white).

CURRENT DATA FILE: B:RAREDEMO.DIF

PLOT OPTIONS

```
                   PLOT AXES: Y
          PLOT GRAPH IN COLOR: Y
                   PEN SPEED: 10
PLOT SYMBOLS AT DATA POINTS: Y
          PLOT SAMPLE LABELS: N
               X-AXIS LABELS: FULL REE
              Y-AXIS MINIMUM: 1
              Y-AXIS MAXIMUM: 1000
                Y-AXIS LABEL: REE/CHONDRITE
                  PLOT TITLE:

Plot, Change, new Data, new File, Quit:
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Figure 2.   The RAREPLOT main menu.

PLOT GRAPH IN COLOR: enter Y to plot data in color or N to plot in a single
    color (black-and-white). When plotting in color, pen number 1 is used to
    plot the axis and labels (a black pen is recommended), then pens 2 through
    6 are used to plot each data set, i.e., data set 1 will be plotted with
    pen 2, data set 2 with pen 3, etc. A notice appears at the bottom of the
    screen indicating how many pens to insert into the pen holders according
    to the option selected.

PEN SPEED: this controls the speed of the pen as it plots; the pen speed
    factor ranges from 1 (slowest) to 10 (fastest). Enter a pen speed factor
    or press RETURN to retain the displayed value. A pen speed factor of 1
    corresponds to approximately 4 cm/sec, and each increment of the pen speed
    factor increases pen speed by about 4 cm/sec up to the maximum pen speed
    of 38.1 cm/sec. The default value for the pen speed factor is 10, which
    is suitable for drafts of plots. A slower pen speed generally produces
    darker, neater lines. A pen speed factor of 1 or 2 is recommended when
    using rapidograph-type drafting pens and mylar drafting film.

PLOT SYMBOLS AT DATA POINTS: press Y or N to select whether symbols will be
    plotted at each data point. The symbols are o, x, □, *, and + (on the HP
    7475A plotter; a different symbol may be plotted rather than the square on
    some models), and will be plotted in that order for each of the up to five
    data sets to be plotted. If you respond no (N) to this prompt a line will
    be drawn without symbols for each data set.

PLOT SAMPLE LABELS: enter Y or N to select whether sample labels will be
    plotted, with their corresponding plot symbols, below the X axis at the
    bottom of the plot (see Fig. 1 for an example). The sample labels are the
    column labels for each data set. If only one set of data is to be
    plotted, a label will not be plotted even if Y is entered in response to
    this prompt. No more than five sample labels may be selected for one pair
    of axes when using multiple plot runs, as the sample labels from the first
    run will be overwritten by those from subsequent plot runs.

X-AXIS LABELS: press the space bar to toggle either FULL REE or PARTIAL REE
    for the X-axis labels, then press RETURN to select. If full REE is
    selected, the abbreviations for all 15 rare earth elements will be plotted
    as X-axis labels; if the partial REE set is selected, only the
    abbreviations for La, Ce, Nd, Sm, Eu, Gd, Tb, Dy, Yb, and Lu will be
    labeled, although all 15 positions will be represented on the X-axis and
    proper spacing between elements will be preserved.

Y-AXIS MINIMUM, Y-AXIS MAXIMUM: enter values for the Y-axis at its origin and
    maximum, or press RETURN to select the automatically scaled values. Only
    whole log scales may be plotted; values will automatically be rounded up
    or down to an even power of ten as appropriate.

Y-AXIS LABEL: enter an appropriate label for the Y-axis, or press RETURN to
    select "REE/CHONDRITE", the default Y-axis label. Press Esc to clear an
    entry from the input line.

PLOT TITLE: enter a plot title, which will be positioned at the top of the
    plot, or press RETURN to retain the currently displayed plot title. Press
    Esc to clear an entry from the input line.

Plot, Change, new Data, new File, Quit: the capitalized letters will be
    colored bright yellow (or become more intense on monochrome screens) when
    this prompt is active, and will return to normal intensity while the
    plotter is working. To plot the data, check to insure that the plot
    parameters are correct and that the plotter is on and loaded with paper
    and pens, then press P to begin plotting. If you wish to change one or
    more parameters before plotting, press C to return to the top of the
    menu. After a plot has been made, press D to enter additional columns
    from the current data file, or press F to load a new data file and select
    data columns. To end the program, press Q.