GEOCHEMICAL DATA ANALYSIS SYSTEM REFERENCE MANUAL

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by J W Sheraton and L Simons

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GEOCHEMICAL DATA ANALYSIS SYSTEM (GDA) - REFERENCE MANUAL

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J.W. Sheraton and L. Simons

ABSTRACT

GDA (Geochemical Data Analysis) is a comprehensive IBM PC-based geochemical data processing system. It is designed to use whole-rock geochemical data retrieved from the ORACLE database, but can be adapted for other databases, or data can be entered into files from the keyboard. The programs are written in FORTRAN 77 (microsoft compiler) and use the Media Cybernetics HALO graphics package for plotting. The system includes facilities for generating plots (histograms, XY plots, triangular plots, spidergrams, etc.), calculating statistical functions (e.g., mean, standard deviation, regression lines, correlation coefficients and cluster analysis) and CIPW norms, printing tables, and carrying out petrogenetic modelling calculations. Plots can be displayed on a PC screen for inspection and editing before being output to a plotter. Other programs allow samples to be assigned to groups for plotting purposes, and allow editing and merging of datafiles.

CONTENTS

1. INTRODUCTION

The geochemical data analysis (GDA) system was developed by Lloyd Simons, a contract programmer with Liveware Computer Services, for the Bureau of Mineral Resources to enable whole-rock geochemical data to be extracted from an ORACLE database and transferred to an IBM PC for analysis and display. The system has been extended to process mineral data, but only the processing of whole-rock analyses is described in this Record. A variety of programs is available to generate plots (histograms, XY plots, triangular plots, spidergrams, etc.), calculate statistical functions, print tables, and carry out petrogenetic modelling calculations. Other programs are used to assign samples to groups for plotting purposes, and edit datafiles.

This manual is intended to assist users when problems arise and to explain the more advanced features of the system. However, it is recommended that new users arrange a demonstration of the software, if possible, and experiment with their own data. A basic knowledge of IBM PCs and MS-DOS is assumed. A summary outlining the use of the system is given in section 13.

1.1 COMMAND SUMMARY

The system consists of several programs on the IBM PC which are invoked by typing the appropriate command:

ORACLE - reads the ASCII file transferred from the database computer and writes the data to an internal (GDA) file for subsequent processing;

ASSIGN - assigns the samples to groups according to logical operations on the descriptive fields; each group is processed as an entity, e.g., all samples in a group are displayed with the same symbol and colour;

GDA - enables sample data to be extracted into datasets either directly or using specified arithmetic expressions or standard operations (e.g., CIPW norms); the datasets can be analysed, previewed on the PC screen, and output to files for later plotting;

PLOT - outputs graphics metafiles (from GDA) to a plotter;

TABLE - generates tables of major and trace elements, CIPW norms, and standard expressions;

STATS - generates correlation matrices and sample statistics;

CLUSTER - Q- and R-mode cluster analysis with dendrogram output;

PETMOD - petrogenetic modelling;
UTIL - utilities that allow editing of GDA files;
OUTGDA - writes contents of a GDA file to an ASCII file for entry to a database (e.g., ORACLE) or for processing by other systems;
ENTMIN - accepts mineral data from the keyboard and writes them out in Oracle format;
PROBE - accepts mineral data on ASCII files from the ANU/BMR Cameca probe and creates an ORACLE format file;
MDA - analysis of mineral data (similar to GDA);
TABMIN - prints tables of mineral data.
The last four of these are used for mineral data, and are not covered in this Record. The system for mineral data is still under development.

1.2 PARAMETER FILES

System parameters, each as elements in spidergrams, are often held on files which can be modified with a word processor (e.g., WORDSTAR). Some files are generated during processing and can also be modified. Care must be taken to preserve the format (logical structure) of the files. The first line of a file must not be changed as it is used to specify the type of file.

1.3 PRINTOUTS

Printout is generated on files that can be printed or input to a word processor. The file is the name of the program with extension .PRN (e.g., ASSIGN.PRN).

1.4 USER INTERFACE

The programs are controlled by selection of options from menus and by typing answers to questions. The standard DOS command interface is used, i.e., no command is processed until the Enter key is pressed, and the backspace key can be used to correct typing errors.

Menus are of the following form:

```
1 = Histogram

2 = XY plot
3 = Triangular plot
4 = Spidergram
Q = Quit
Option [1-4,Q] (exit):
```

where the option is chosen by typing the related number (followed by Enter). Sometimes a hierarchy of menus is presented, and just pressing the Enter key will cause control to return to the previous menu (until the first is reached).

Questions and commands are of the following form, e.g.,

```
Type marker size [0.1-2.0cm] (0.5):
Do you want to display sample names [Y/N] (Y)?
Arithmetic expression [?=help]:
```

where general information, range of values, etc., are given in [] and any default that will be taken if just the Enter key is pressed is given in ( ).

Each answer is checked by the system, and if invalid a message may appear and the question is repeated.

Values must be given within any indicated range, and a decimal point should be included if (and only if) the indicated range of default values shows it.

1.5 SOFTWARE

All the software is written in Microsoft FORTRAN 77 (version 4.0). Media Cybernetics HALO 88 is used for graphics to provide support for HP plotters and several displays (EGA, Hercules, and VGA, but note that earlier versions of HALO do not support VGA).

1.6 HARDWARE REQUIREMENTS

An IBM PC or compatible is required with 640K RAM, a 10 megabyte hard disk (the actual programs require about 3 mb), and a Hercules, EGA, or VGA colour graphics card. An HP compatible plotter is required for hardcopy graphics and a printer for reports.

1.7 GDA FILE

The software operates on sets of samples held in geochemical (GDA) files. Each sample is one random access record in the file, and is identified by its sample number.

The data for each sample are in two parts. The first part consists of descriptive data, of which only the sample number is mandatory. Other descriptive fields could be locality, stratigraphic unit, lithology, originator, etc. Descriptions can be up to 32 characters. Descriptive fields are used to assign samples to groups for display. The other part consists of concentrations for a defined set of elements. Major elements (as oxides) are given in weight percent, while trace elements are given in parts per million (PPM). Zero is held if there is no value for an element. Where an element was not detected, a value of the negative of the detection limit is stored (half the detection limit is used in most processing).

The names of the descriptive and element fields are up to 10 characters long and can generally be anything, but the sample number must have the name 'SAMPNO' and norm and modelling programs require conventional element names to be used.

The data will usually be extracted from a data base or will be generated by analysis equipment, and must be in external Oracle database format before they can be made into a GDA file using the ORACLE program. Alternatively, data can be typed directly into a GDA file with the utilities program (UTIL), which can also be used to edit GDA files. GDA files are usually given names with the extension .GDA.

Before data in a GDA file can be processed, samples must be assigned to groups using the ASSIGN program. Finally, the various data-processing

programs (GDA, PLOT, TABLE, STATS, CLUSTER, and PETMOD) can be used.

2. INSTALLATION

The software is provided on several floppy disks. The GDA system may be built up from the FORTRAN source code if Microsoft FORTRAN 77 and HALO are also installed, and details are given in Appendix B. Alternatively, if the compiled version is available, it is only necessary to follow these steps:

. Set up a directory \gda\ on the hard disk by typing mkdir gda;

. Copy the contents of all the floppy disks to the gda directory;

. Rename the screen driver file to be SCREEN.DEV; the driver files are:

EGA.DEV = the EGA driver
HERC.DEV = the Hercules driver
VGA.DEV = the VGA driver;

the other files can be deleted;

. Edit the file SITE.DEF with a word processor to define the plotter that is to be used.

A sample file is:

```
Site Definition File        SITE.DEF
8 Number of pens, the (red,green,blue) values & names follow
1 1.00 1.00 1.00 Black                White on screen
2 1.00 0.00 0.00 Red
3 0.00 1.00 0.00 Green
4 0.00 0.00 1.00 Blue
5 1.00 1.00 0.00 Yellow
6 1.00 0.00 1.00 Purple
7 1.00 0.50 0.00 Brown
8 1.00 0.50 0.50 Pink
HP7550     The HP plotter model
  0        The communications port, 0=port1, 1=port2
  0        Autofeed, 1=7550 autofeed, 0=none
 10        Speed in cm/second
40.4       Plotter page width in cm    A3 page, assumed in SW
28.5       "       "   height
10760      Offline plotter page width in HPGL address units - 400*size
07600       "       "       "   height    "     "       "
EGA        Graphics card
0.00 0.00 0.00   Screen background colour
```

In this example the offline plotter page size specified is A4. The settings for an A3 Plotter are 15410 and 10870, which actually give a slightly reduced plot. (It was not found to be possible to produce an undistorted, full-size plot.)

The HP plotter models supported and switch settings for serial ports are (see HALO manual):

HP7475: s2=0, s1=0, D, US, A4, b4=1, b3=0, b2=1, b0=0

HP7470: s2=0, s1=0, D, US, b4=1, b3=0, b2=1, b0=0

HP7550: enhanced, bypass off, Xon/Xoff, Direct, Remote, standalone, full duplex, 9600 baud, parity 8 bits off, monitor mode off

HP7510: 9600 baud, no parity, full duplex, 8 data bits, no auto-disc, direct connection, standalone, bypass off, remote mode, Xon/Xoff handshake

The file PLOT.BAT sets up the communication port. If COM2 is used, the file will have to be modified

Compatible plotters will probably work with the HP7550 driver as long as they are connected at 9600 baud.

The table of pens and their colours should be set up to agree with the actual plotter pens so plots previewed on a colour screen will agree (or the pens could be installed in the plotter in the correct order). Colours are given as (red,green,blue) triples. The plotter model number is the same as the name of the translator program. The plotter page size must be correct if actual sizes are to be used when specifying plot parameters. The software is set up with defaults for A3 paper.

The other plotter translator files (HP????.EXE) can be deleted.

A file TSTGDA.DAT, which is geochemical data in oracle format, is provided for use when trying out the system.

3. ORACLE

Data are entered into the system as 80 character records in Oracle format (ASCII files). This program transfers the data to an internal (GDA) file for subsequent processing. The following example of an input file is for intrusive rocks from the Mount Isa region (actually part of TSTGDA.DAT), extracted from the BMR ORACLE database:

```
SQL>SPOOL TEMP1;
 2   SET PAGE SIZE 50 000;
 3   SELECT
 4   STATE, REGION, LOCALITY, SAMPNO, STRATGROUP, STRATUNIT, MAPSYMBOL,
 5   LITHOLOGY, MAPNAME, GRIDREF, DRILLHOLE, DEPTH, AGE, BIBLIOREF,
 6   ORIGINATOR, OTHERDATA, SIO2, TIO2, AL2O3, FE2O3, FEO, MNO, MGO, CAO,
 7   NA2O, K2O, P2O5, H2OPLUS, H2OMIN, CO2, Ba, Li, Rb, Sr, Pb, Th, U,
 8   Zr, Nb, Y, La, Ce, Nd, Sc, V, Cr, Mn, Co, Ni,  Cu,  Zn, Sn, W,
 9   Mo, Ga, Ars, S, C, F, Cl, B, Ag, Au, Hg, Bi, Ge, Xa, Xb, Xc,
10   Xd, Be, Br, LOI (or SELECT * to select all fields)
11   FROM READCHEM
12   WHERE REGION = 'Mount Isa'; (or specify other logic)
```

```
STATE      REGION                LOCALITY              SAMPNO
---------- --------------------- --------------------- --------------------
STRATGROUP                       STRATUNIT                        MAPSYMBOL
-------------------------------- -------------------------------- ----------
LITHOLOGY              MAPNAME                GRIDREF    DRILLHOLE  DEPTH
---------------------- ---------------------- ---------- ---------- ----------
AGE        BIBLIOREF  ORIGINATOR             OTHERDATA                SIO2  TIO2
---------- ---------- --------------------- --------------------- ----- -----
AL2O3 FE2O3 FEO   MNO   MGO   CAO   NA2O  K2O   P2O5  H2OPL H2OMI CO2   BA
----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- -----
LI    RB    SR    PB    TH    U     ZR    NB    Y     LA    CE    ND    SC
----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- -----
V     CR    MN    CO    NI    CU    ZN    SN    W     MO    GA    ARS   S
----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- -----
C     F     CL    B     AG    AU    HG    BI    GE    XA    XB    XC    XD
----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- ----- -----
BE    BR    LOI
----- ----- -----
Qld        Mount Isa                                      78206000
Kalkadoon Batholith              Kalkadoon G.diorite
granodiorite                Alsace                910153
           Wyborn      L. Wyborn                   1/1                    67.57  0.35
15.88  0.52  2.26  0.04  0.50  3.15  3.14  4.67  0.07  0.61  0.07  0.09  1268

    7   192   287    15    21     3   207    11    29    71   127    54     7
   20     7           5     2     9    35     4                16     3
```

Qld Mount Isa 78206001
Tewinga Group Leichhardt Metamorph.
xenolith Alsace 911152
Wyborn L. Wyborn 1/1 67.23 0.89
13.00 1.35 4.93 0.04 0.67 2.40 3.04 4.98 0.19 0.61 0.18 0.22 822
6 175 71 16 24 6 428 25 65 71 137 66 10
27 8 10 5 26 15 9 18 2

Qld Mount Isa 78206002
Tewinga Group Leichhardt Metamorph.
xenolith Alsace 910151
Wyborn L. Wyborn 1/1 70.22 0.40
14.03 1.69 2.39 0.05 0.45 2.84 3.16 3.77 0.08 0.50 0.08 0.04 830
5 159 171 28 20 3 293 11 34 53 101 45 9
15 10 8 3 6 58 -2 18 1

Qld Mount Isa 78206003
Kalkadoon Batholith Kalkadoon G.diorite
syenogranite Alsace 899165
Wyborn L. Wyborn 1/1 76.30 0.10
12.25 0.20 1.03 0.02 0.21 0.78 3.04 5.07 -0.01 0.46 0.07 0.08 288
3 203 67 23 29 7 111 10 29 35 68 32 -2
2 7 3 3 8 32 3 14 4

Qld Mount Isa 78206004
Kalkadoon Batholith Kalkadoon G.diorite
monzogranite Alsace 905161
Wyborn L. Wyborn 1/1 75.05 0.13
13.14 0.40 1.02 0.02 0.15 1.36 2.93 4.99 -0.01 0.55 0.05 0.02 389
6 242 108 31 26 6 126 12 33 42 83 35 -2
3 7 4 3 5 12 4 15 -1

Qld Mount Isa 78206005
Kalkadoon Batholith Kalkadoon G.diorite
monzogranite Alsace 906157
Wyborn L. Wyborn 1/1 71.60 0.19
14.64 0.46 1.30 0.03 0.21 2.02 3.29 5.03 0.02 0.53 0.06 0.03 722
9 237 175 28 25 3 143 10 28 53 98 43 3
6 6 4 1 3 34 3 16 -1

Qld Mount Isa 78206006
Kalkadoon Batholith Kalkadoon G.diorite
monzogranite Alsace 909146
Wyborn L. Wyborn 1/1 70.69 0.31
14.66 0.46 2.05 0.04 0.44 2.41 2.84 4.74 0.06 0.62 0.07 0.06 774
8 204 208 23 24 6 168 11 31 66 117 49 3
16 8 5 2 5 26 7 16 1

```
Qld          Mount Isa                                          78206011
Naraku Batholith                    Capsize g.diorite
tonalite                    Quamby                  182552
                Wyborn      L. Wyborn                1/18                          65.08  0.58
15.32  2.54  3.39  0.04  1.48  3.63  4.26  1.95  0.20  0.71  0.14  0.07   475
   11    94   231     4    27     4   359    15    41    71   118          12
   88    10          15    11    18    19     2          -3    18     1

Qld          Mount Isa                                          78206012
Naraku Batholith                    Capsize g.diorite
tonalite                    Quamby                  175545
                Wyborn      L. Wyborn                1/18                          65.59  0.60
15.20  2.27  3.31  0.04  1.41  3.64  3.84  2.07  0.18  0.95  0.11  0.06   749
   12    80   259    14    31     3   380    15    46   104   171          12
   75    10          15     8    22    23     2          -3    18    -1
```

9 records selected

SQL >SPOOL OFF;.

Any data can be entered providing they are in this form, i.e., the ORACLE data base system does not have to be used.

The file must consist of records of up to 80 characters.
The front of the file can have garbage records, such as the Oracle select statement in the above example, and a few surplus records (less than the number in a sample) can be on the end.

The first significant records describe the fields in the file, and paired with each record is another with ----- indicating the maximum number of characters in the field.
The actual data records follow, and must follow the header records format.

The file FIX.DEF is used to change the names of the elements in the data. There are restrictions on the characters that can be used in Oracle, and the CIPW norm routine, etc. expects definite names (as in REPORT.RPT) so any differences should be corrected via this file.

A sample file is:

```
Oracle element name corrections FIX.DEF
03
H2OPL      H2O+
H2OMI      H2O-
ARS        AS
```

Restrictions are:

the maximum field size for descriptive fields is 32 characters, and for

concentrations is 20 characters. Descriptive fields that are too long are truncated. Five digits are usually enough for concentrations, but ten is probably preferable with the decimal point being included.
Concentrations can be given as decimal values or right-justified integers.
The descriptive fields must all be at the beginning of each record.
The field SAMPNO must be in the descriptive fields to give an identifier for each sample. The additional field ANALNO is usually used for mineral analyses as there could be several analyses for each sample.
The field SIO2 indicates the first element concentration field, i.e., it follows the descriptive fields, must be present, and precedes all other concentration data. Any subsequent fields are taken as containing numerical data. With this proviso, the actual order within each set of fields (i.e., descriptive and concentration) is immaterial.
A concentration of zero means that there is no value for that element.
When an element concentration is below the detection limit, the value given is the negative of the detection limit. The value used in processing will be half the positive value.
All field names are held internally in upper case to simplify comparisons, but can be redefined for the report programs.

The program is run by typing ORACLE.

You must provide the name of the oracle file to be read in, e.g.,
BKHILL.ORC A:JUNE.LIS

You must also give the name of the internal file generated. The default CURRENT.GDA is also the default for other programs.

Often the data file will have been transferred to the PC over a network and there could be corrupted records due to transmission errors.
There is a choice of either having concentrations set to zero on read errors or being asked to type in correct values.

4. ASSIGN

The first processing step is to assign the samples in the GDA file to groups. A group is a logical set of samples which will be displayed with all samples within it having the same symbol. At least some of the samples on a GDA file must be assigned to groups before plots can be generated.

Samples are assigned to a group according to logical operations on the descriptive fields (e.g., region, locality, lithology, etc.) on the file.

The program is run by typing ASSIGN. Option 1 on the main menu is then selected to define the group logic. A global selection can be specified to provide overall criteria for accepting or rejecting samples; if not specified all samples will be considered.

The following must be specified for each group:

- The group name (max. of 20 characters), which appears on the legend and on menus for selection of group parameters such as the symbol;

- Logical expressions to assign the samples to the group.

The logic is typed in as lines, where each line is an 'or' condition. A maximum of 10 lines can be specified. Each line consists of one or more logical tests separated by 'and' conditions. The tests are given as the descriptive field name compared to a text string. Operations are

```
== equality
!= inequality
&& and.
```

For example, granites from Broken Hill, shales from Sydney, and gold from anywhere could have the following logic:

```
LITH==GRANITE && LOCATION == BROKEN
Lithology==SHALE && LOCATI == SYD
liTH == GOLD
```

Note that upper and lower case are taken as the same in the comparison. Both the descriptive field name and text string can be shortened (but must be unique) and the text comparison will be anywhere in the data field. It may be useful to have some extra information in the 'otherdata' field to aid assignment of samples into groups. For example, mafic dyke suites with different geochemical characteristics may already be classified as Group 1, 2, etc., or garnet gneisses from the Rauer Islands may be identified by 'Rauer Gt' (see example below).

After the logic has been specified for each group the file is processed and the samples assigned to groups (option 12). If a sample is assigned to more than one group, the first assignment is used and a message appears. All samples may be assigned to one group, if desired (option 13).

The logic and group names can be re-entered if an error has been made. Items 2-9 on the menu allow editing of the logic. The logic can be stored on a file (option 10) and retrieved for modification and re-use. This should always be done when samples are first assigned to groups, as subsequent use of ASSIGN to change or edit group logic results in loss of the previous logic. The file can be modified with a word processor, but the number of records in the file and the header record must not be changed (i.e., be careful!). It is possible to set up several logic files for a given GDA file but the samples must be re-assigned if a different logic file is to be used.

The menu is as follows:

(1) Define new set of groups.
(2) List global logic.
(3) Change global logic.
(4) List group titles.
(5) Change group titles.
(6) List logic for groups.
(7) Change logic for groups.
(8) Delete groups.
(9) Define new groups.
(10) Save logic on file (this should be done each time new logic is specified).

(11) Restore logic from file.

(12) Assign analyses to groups (using the previously specified logic).

(13) Assign all analyses to group 1.

An example of a logic file (for metamorphic rocks from Antarctica) is:

```
Global logic
Process all records

Group number 1
Rauer Opx gneiss
Other==Rauer Op

Group number 2
Rauer Gt gneiss
Other==Rauer Gt

Group number 3
Prydz Opx gneiss
other==Prydz Op

Group number 4
Prydz Gt gneiss
other==Prydz Gt

Group number 5
Granite
lithol==Granite

Group number 6
Pelite
lithol==pelite

End-of-data
```

Assignment of samples into the specified groups may be printed out from the file ASSIGN.PRN. An example using the above logic is given below.

ASSIGN SAMPLES TO GROUPS

Analysis 81285103	assigned to group 1		
Analysis 81285104	assigned to group 2		
Analysis 81285107	not assigned		
Analysis 81285110	assigned to group 2		
Analysis 81285112	assigned to group 2		
Analysis 81285114	assigned to group 2		
Analysis 81285114	*** group conflict ***	2	5
Analysis 81285115	assigned to group 1		
Analysis 81285115	*** group conflict ***	1	5
Analysis 81285116	not assigned		
Analysis 81285118	assigned to group 2		
Analysis 81285119	assigned to group 1		
Analysis 81285120	assigned to group 1		
Analysis 81285123	assigned to group 2		
Analysis 81285124	assigned to group 1		
Analysis 81285125	assigned to group 1		
Analysis 81285127	assigned to group 1		
Analysis 81285128	assigned to group 2		
Analysis 81285131	assigned to group 1		
Analysis 81285133	assigned to group 1		
Analysis 81285133	*** group conflict ***	1	5
Analysis 81285134	assigned to group 2		
Analysis 81285134	*** group conflict ***	2	5
Analysis 81285135	assigned to group 2		
Analysis 81285138	assigned to group 2		
Analysis 81285140	not assigned		
Analysis 81285141	not assigned		
Analysis 81285143	assigned to group 1		
Analysis 81285145	assigned to group 4		
Analysis 81285147	assigned to group 6		
Analysis 81285148	assigned to group 6		
Analysis 81285150	assigned to group 5		
Analysis 81285151	assigned to group 5		
Analysis 81285155	assigned to group 6		
Analysis 81285156	assigned to group 4		
Analysis 81285158	assigned to group 4		
Analysis 81285207	assigned to group 4		
Analysis 81285208	assigned to group 6		
Analysis 81285211	assigned to group 4		
Analysis 81285214	assigned to group 6		
Analysis 81285218	assigned to group 6		
Analysis 81285219	assigned to group 6		
Analysis 81285223	assigned to group 4		
Analysis 81285224	assigned to group 6		
Analysis 81285228	assigned to group 6		
Analysis 81285229	assigned to group 4		
Analysis 81285269	assigned to group 4		
Analysis 81285270	assigned to group 6		
Analysis 81285271	assigned to group 6		
Analysis 81285272	assigned to group 4		
Analysis 81285273	assigned to group 6		
Analysis 81285275	assigned to group 3		
Analysis 81285276	assigned to group 4		
Analysis 81285291	assigned to group 4		
Analysis 81285295	assigned to group 4		
Analysis 81285298	assigned to group 4		
Analysis 81285298	*** group conflict ***	4	5
Analysis 81285300	assigned to group 4		
Analysis 81285302	assigned to group 4		
Analysis 81285304	assigned to group 6		

Analysis 81285306	assigned to group 4
Analysis 81285309	assigned to group 6
Analysis 81285329	assigned to group 6
Analysis 81285330	assigned to group 4
Analysis 81285332	assigned to group 6
Analysis 81285333	assigned to group 6
Analysis 81285336	assigned to group 6
Analysis 81285341	assigned to group 4
Analysis 81285342	assigned to group 6
Analysis 81285346	assigned to group 4
Analysis 81285347	assigned to group 5
Analysis 81285352	assigned to group 6
Analysis 81285356	assigned to group 6
Analysis 81285375	assigned to group 5
Analysis 81285376	assigned to group 5
Analysis 81285378	assigned to group 5
Analysis 81285380	assigned to group 5
Analysis 81285381	assigned to group 5
Analysis 81285383	assigned to group 4
Analysis 81285385	assigned to group 4
Analysis 81285388	assigned to group 4
Analysis 81285389	assigned to group 3
Analysis 81285391	assigned to group 3
Analysis 81285392	assigned to group 3
Analysis 81285395	assigned to group 3
Analysis 81285397	assigned to group 5
Analysis 81285399	assigned to group 5
Analysis 81285401	assigned to group 4
Analysis 81285405	assigned to group 4

Group	No samples
1	10
2	10
3	5
4	24
5	10
6	21
None	4

5. GDA (and BIGGDA)

This is the main program which allows data to be plotted on various types of graph (XY, XYZ, histogram, spidergram). A second version (BIGGDA) allows more samples (>1000, <2000) to be plotted, although only 4 datasets (e.g., elements) can be extracted at once, and least squares lines cannot be calculated. These programs are run by typing GDA or BIGGDA, as appropriate. A GDA file name (as generated in the ORACLE program) must then be specified.

5.1 DATA EXTRACTION

The first step is to extract data (element concentrations, normative minerals, or expressions such as ratios) to be plotted. Up to 11 such datasets may be extracted at once. Items 1-4 on the GDA menu are used to extract data into datasets 1-11. The name of the GDA file (i.e., datafile) must be given.

(1) Extract Values for Standard Expressions

Standard arithmetic expressions may be stored on a file for subsequent use. The default file (STDEXP.DEF) includes such expressions as mg value, total Fe as FeO, ASI, K/Rb and Ga/Al, any of which may be selected and assigned to given datasets (see Appendix C). Other expressions may be added, or other files set up to include any required expressions, but note that the format of the file must be followed. The first record is fixed ('Standard Arithmetic Expressions') and specifies the type of file, and each entry is a single line arithmetic expression followed by the label to be used for display.

(2) Extract Values for Typed-In Expressions

Individual element concentrations (e.g., SiO2, Rb) or expressions (e.g., Ce/Y, 8301 * K20/Rb) may be retrieved by typing in directly on the keyboard and assigning to datasets 1-11.

Operators are:

+ addition
- subtraction
* multiplication
/ division
> greater than or equal to
< less than or equal to
** power

Functions available are:

LOG10	common logarithm
LOG	natural logarithm
SQRT	Square root
ABS	absolute value
EXP	exponential
AINT	truncation
TAN	tangent
ATAN	arc tangent
SIN	sine
COS	cosine
SINH	hyperbolic sine
COSH	hyperbolic cosine

Datasets are referred to by two characters strings '$n' (e.g., $2 is dataset number 2). Hence, datasets can be used to hold intermediate values.

Pi is referred to as PI. Expressions are evaluated left to right, * and / before + and -. Parentheses should be used to ensure there are no ambiguities.

(3) Extract Standard Datasets

The default file (STDSET.DEF) includes 11 major elements, 11 trace elements, and values for various triangular plots, such as AFM, ACF and Ti-Zr-Y diagrams (see Appendix C). Other 'Standard Dataset

Definitions' files may be set up, provided the file format is adhered to. Each specification starts with a title that will appear in the menu and as the plot title, and a two digit record that gives the number of datasets. There follow records giving the plotting labels for each dataset, and then records giving the arithmetic expressions for each dataset.

Values for triangular plots are assigned to datasets 1-3. Note that values will replace those previously assigned to the same dataset.

(4) Extract CIPW Norm Values

Values for standard CIPW normative minerals, calculated using the method of Kelsey (1965), may be extracted, together with normative expressions (differentiation index, colour index, Pl = Ab + An, 100 An/(Ab + An), 100 An/(Ab^ + An), Ab^ = Ab + 1.85 Ne, Q" = Q + 0.299 En + 0.228Fs, Ol^ = Ol + 0.701En + 0.772FS, Ne^ = Ne + 0.542Ab, Q^ = Q" + 0.458Ab, mg number). All normative minerals and derived expressions are weight percent values. Note that the normative basalt tetrahedron (Di-Fo-Ne-Q) of Yoder & Tilley (1962) was also based on weight percent norms. However, such values differ only slightly from molecular (i.e., cation) norms (see Irvine & Baragar, 1971).

It is necessary to specify various parameters, comprising:

1. Incorporate trace element data into calculations.
2. Recalculate to anhydrous conditions.
3. Normalise analyses.
4. Specify initial $Fe^{2}/(Fe^{2}+ Fe^{3})$ ratio.
5. Ignore CO_2.
6. Calculate CO_2 first as cancrinite rather than calcite.

If other arithmetic expressions involving normative minerals are required, the minerals are first assigned to datasets, then the expression is entered into a subsequent dataset from the keyboard as a typed-in expression (see 2 above). For example, to plot Hy + Di, first assign Hy and Di to datasets 1 and 2 (say), then assign $1 + $2

to dataset 3. ($1 refers to dataset 1, etc.). Datasets may similarly be used to hold any intermediate values. Note that expressions involving normative minerals will be evaluated and plotted if the value for one or more minerals is zero, but not expressions involving only element concentrations. Thus, Hy + Di will be plotted if Hy or Di (but not both) = 0, whereas Ce + Y will not be plotted if either Ce or Y = 0.

5.2 DEFINING PLOT PARAMETERS

Item 6 on the GDA menu ('Define main plot parameters') is used to allocate symbols, pen colours, and linetypes to sample groups, and to define symbol, text, and axis dimensions. Commonly the default parameters may be adequate, but these may be changed and the plot parameters stored on a file for subsequent retrieval and re-use. Different parameters may be required for display on screens and on plotters.

The various optional parameters can be allocated using the following menu. Default values are given in brackets.

(1) Retrieve plot parameters (from file).
(2) Change title text height (1.5cm).
(3) Change axes labels text height (1.0 cm).
(4) Change sample numbers text height (1.0cm; also used for added plot point labels and text).
(5) Change symbol height (0.5 cm).
(6) Change axes tick height (1.0 cm).
(7) Change font (no. 5).
(8) Change group pens.
(9) Change group symbols.
(10) Change group linetypes (1).
(11) Change axes pen (1).
(12) Change titles pen (1).
(13) Change histogram pen (1).
(14) Change plot title.
(15) Change legend symbol and text height (1.0).
(16) Change axes lengths (X = 25.0cm; Y = 20.0cm).
(17) Store plot parameters (on file).

An example of a plot parameters file is given below. Note that only symbols and pen colours for the 6 assigned groups (1-6) have been changed; parameters for the remaining (un-assigned) groups are the default values. Normally the format will not be of interest as it will not be necessary to edit such a file.

Plot Parameters

```
1          12          1          1 Group Symbol Pen Linetype
2           2          1          1 Group Symbol Pen Linetype
3          12          2          1 Group Symbol Pen Linetype
4           2          2          1 Group symbol Pen Linetype
5           3          3          1 Group Symbol Pen Linetype
6           6          4          1 Group Symbol Pen Linetype
7           7          7          1 Group Symbol Pen Linetype
8           8          8          1 Group Symbol Pen Linetype
9           9          1          1 Group Symbol Pen Linetype
10         10          2          1 Group Symbol Pen Linetype
11         11          3          1 Group Symbol Pen Linetype
12         12          4          1 Group Symbol Pen Linetype
13         13          5          1 Group Symbol Pen Linetype
14         14          6          1 Group Symbol Pen Linetype
15         15          7          1 Group Symbol Pen Linetype
16          1          8          1 Group Symbol Pen Linetype
17          2          1          1 Group Symbol Pen Linetype
18          3          2          1 Group Symbol Pen Linetype
19          4          3          1 Group Symbol Pen Linetype
20          5          4          1 Group Symbol Pen Linetype
21          6          5          1 Group Symbol Pen Linetype
22          7          6          1 Group Symbol Pen Linetype
23          8          7          1 Group Symbol Pen Linetype
24          9          8          1 Group Symbol Pen Linetype
25         10          1          1 Group Symbol Pen Linetype
26         11          2          1 Group Symbol Pen Linetype
27         12          3          1 Group Symbol Pen Linetype
28         13          4          1 Group Symbol Pen Linetype
29         14          5          1 Group Symbol Pen Linetype
30         15          6          1 Group Symbol Pen Linetype
31          1          7          1 Group Symbol Pen Linetype
32          2          8          1 Group Symbol Pen Linetype
33          3          1          1 Group Symbol Pen Linetype
34          4          2          1 Group Symbol Pen Linetype
35          5          3          1 Group Symbol Pen Linetype
36          6          4          1 Group Symbol Pen Linetype
37          7          5          1 Group Symbol Pen Linetype
38          8          6          1 Group Symbol Pen Linetype
39          9          7          1 Group Symbol Pen Linetype
40         10          8          1 Group Symbol Pen Linetype
41         11          1          1 Group Symbol Pen Linetype
42         12          2          1 Group Symbol Pen Linetype
43         13          3          1 Group Symbol Pen Linetype
44         14          4          1 Group Symbol Pen Linetype
45         15          5          1 Group Symbol Pen Linetype
46          1          6          1 Group Symbol Pen Linetype
47          2          7          1 Group Symbol Pen Linetype
```

```
48          3          8          1 Group Symbol Pen Linetype
49          4          1          1 Group Symbol Pen Linetype
50          5          2          1 Group Symbol Pen Linetype

 5    1.5000    1.0000     1.0000 Font Text height
 .5000 symbol size
1.0000 Tick height
     1          1       1 Axes and Titles and histogram pens
1.0000 Legend symbol and text height
25.0000     20.0000 Axes lengths
```

There are choices of up to 8 pens (depending on the type of plotter), 15 symbols, 6 linetypes (for spidergrams), and 19 fonts, all of which may be displayed (Figures 2-4). As default values for these, pen 1 and symbol 1 are assigned to group 1, pen 2 and symbol 2 to group 2, and so on. Pens and symbols assigned to each group may be checked by displaying the legend (Figure 1). The default linetype for all groups is 1 (solid line); note that the linetypes as displayed on the screen are slightly different from those used by the plotter (they are defined in the HALO package).

The default axis lengths (25 x 20 cm) produce a plot of that size on the plotter, and a somewhat reduced plot on the screen. The size and shape of the final plot (triangular plots excepted) may be changed by changing the axis lengths, but note that the maximum plot size (including axis labels) for an A3 page plotter is about 40 x 28 cm and that such a plot size would overflow the screen. However, this option can be useful in arranging more than one plot on a single page (see under PLOT). The default symbol and text sizes are appropriate if 4 plots per page are output to the plotter (see under PLOT), but may need changing if this is not the case. The numbers of axis labels and ticks on each axis are set automatically and cannot be selected by the user. However, the numbers will be reduced if plots are stacked or reduced in size. It is possible to set the tick size to zero, and add the required number of ticks by hand.

FIG. 1. Legend.

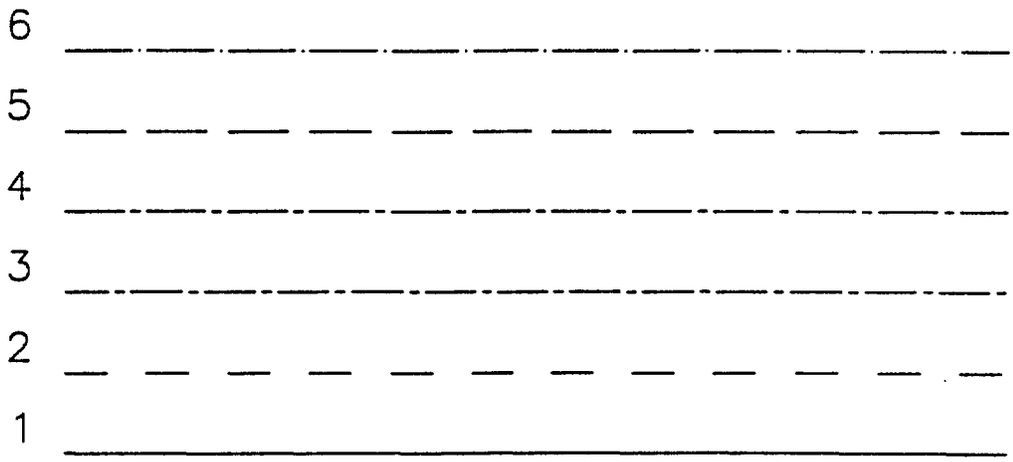


FIG. 2. Linetypes.

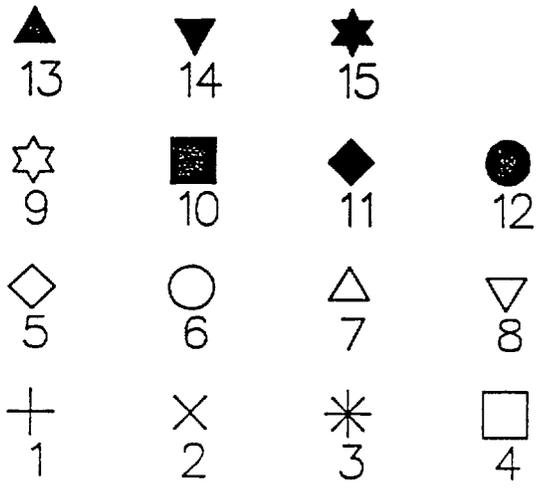


FIG. 3. Symbols.

Font no 1	*Font no 2*	Font no 3
1234567890	1234567890	1234567890
uvwxyz&*{]	*uvwxyz&*{]*	uvwxyz&*{]
UVWXYZ	*UVWXYZ*	UVWXYZ
klmnopqrst	*klmnopqrst*	klmnopqrst
KLMNOPQRST	*KLMNOPQRST*	KLMNOPQRST
abcdefghij	*abcdefghij*	abcdefghij
ABCDEFGHIJ	*ABCDEFGHIJ*	ABCDEFGHIJ

Font no 4	Font no 5	Font no 6
1234567890	1234567890	1234567890
uvwxyz&{]*	uvwxyz&*{]	uvwxyz&*{]
UVWXYZ	UVWXYZ	UVWXYZ
klmnopqrst	klmnopqrst	klmnopqrst
KLMNOPQRST	KLMNOPQRST	KLMNOPQRST
abcdefghij	abcdefghij	abcdefghij
ABCDEFGHIJ	ABCDEFGHIJ	ABCDEFGHIJ

Φοντ νο 7	*Font no 8*	Font no 9
1234567890	*1234567890*	1234567890
νωξψζ(ϑ[]	*uvwxyz&*{]*	uvwxyz&*{]
Τ∝ΩΞΨΖ	*UVWXYZ*	UVWXYZ
κλμνοπϑρστ	*klmnopqrst*	klmnopqrst
ΚΜΝΟΠΘΧΣΤ	*KLMNOPQRST*	KLMNOPQRST
αβηδεφγχι	*abcdefghij*	abcdefghij
ΑΒΗΔΕΦΓΙΛ	*ABCDEFGHIJ*	ABCDEFGHIJ

FIG. 4

Font no 10
1234567890
uvwxyz&*[]
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

Font no 11
1234567890
uvwxyz&*
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

Font no 12
1234567890
uvwxyz&*
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

Font no 13
1234567890
uvwxyz&*
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

Font no 14
1234567890
uvwxyz&*
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

Font no 15
1234567890
uvwxyz&*
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

Font no 16
1234567890
uvwxyz&*
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

Font no 17
1234567890
uvwxyz&*
UVWXYZ
klmnopqrst
KLMNOPQRST
abcdefghij
ABCDEFGHIJ

F 18
1234567890
&
UVWXYZ
KLMNOPQRST
ABCDEFGHIJ

FIG. 4 (cont.)

5.3 PLOTTING OF DATA

Data extracted into datasets can be plotted on various types of diagram, namely datasets display, histograms, XY plots, triangular plots, and spidergrams. Plot legends (i,e,, symbols and group names) may also be displayed. These options are called up using items 7 - 12 on the GDA menu. Text may be added to any plot, and some types of plot include statistical functions such as least-squares fits, regression lines, means, and standard deviations, which may be displayed if required. Least-squares lines are calculated assuming errors in both X and Y . In contrast, regression curves assume that there are no errors in the X-axis variable, i.e., X is the independent variable and Y the dependent variable. Further details are given by Williamson (1968) and Brooks & others (1972). Normally, plots are initially displayed on the PC screen to allow inspection and editing before being written to metafiles for later output to a plotter using the PLOT program. Examples of the various plots available are shown below.

(7) Display Datasets

This enables one or more datasets to be displayed on an XY plot of value against sample order in the dataset. Each sample group is displayed sequentially, using the appropriate symbol and pen colour. Either a single dataset (e.g., element) may be displayed, or plots of up to 10 datasets may be stacked.

The menu is as follows:

(1) Display (either on screen or metafile; plot number (1-99) must be specified in latter case).

(2) Select datasets (e.g., elements) for display (if more than one is selected, plots will be stacked).

(3) Change plot title.

(4) Change axes titles (for any selected dataset).

(5) Display sample numbers (on plot).

(6) Set axes extremes to data range plus 20%.

(7) Set axes extremes to nice limits (this is the default which selects a logical whole-number range for each axis, depending on which groups are selected for display).

(8) Set axes extremes to typed-in values (any values may be selected, but note that they will also apply to histograms and XY plots (but not triangular plots)).

(9) Set log or linear axes (for any selected dataset).

(10) Define pen for mean lines (1 of up to 8 colours; displays means for all groups selected for display in 13).

(11) Define pen for median lines (as 10).

(12) Define pen for standard deviation lines (as 10).

(13) Select groups to be displayed (any or all assigned groups may be displayed on each plot).

(14) Specify additional plot points and/or text (additional plot points or text, such as a legend, may be added to previously selected plots via the keyboard. The following must be given:

1. X, Y co-ordinates (separated by a comma; previously specified points or text will be deleted if no values are entered here; co-ordinates outside the plotting area are permissible).

2. Pen number.

3. Symbol number (if none is given, only text will be output).

4. Text (e.g,, sample number or a legend; 0 - 25 characters).

5. Y - axis dataset (this number must be specified for each extra point or text required; for stacked plots, points or text may be added to any plot by specifying the appropriate dataset).

Note that the given XY co-ordinates define the centre of the symbol or, if no symbol is specified, the bottom of the first character of text. All added points or text required for a given plot (either single or stacked) must be specified in one operation (as previously added points will be replaced when this option (14) is selected a second time); the maximum is 20 extra points and/or text lines).

(15) List statistics (includes minimum, maximum, mean, median, standard deviation, skewness, and kurtosis; calculated for all samples in the selected groups and for selected datasets; if log axes are selected, statistics will be calculated using natural log values).

The statistics are displayed, and are also listed on a file GDA.PRN, which may subsequently be printed.

(8) Display Histograms

Histograms of three types may be displayed - for single datasets, stacked for up to 10 datasets, or stacked for selected groups for a single dataset (see item 13). The menu is similar to that for display of datasets:

(1) Display (on screen or metafile 1-99).

(2) Select datasets (e.g., elements) for display.

(3) Change plot title.

(4) Change axes titles.

(5) Set axes extremes to data range plus 20%.

(6) Set axes extremes to nice limits.

(7) Set axes extremes to typed-in values.

(8) Define histogram box width.

(9) Define pen for mean lines.

(10) Define pen for median lines

(11) Define pen for standard deviation lines.

(12) Select groups to be displayed.

(13) Select histogram type:

1. Single element (for all selected groups).

2. Stacked for selected datasets (for all selected groups).

3. Stacked groups for one dataset (each selected group is plotted separately with group numbers at right).

(14) Specify additional plot points and/or text (for histograms, this option is mainly useful for adding text, such as a legend, to a previously selected plot:

1. X, Y co-ordinates (separated by a comma; if no values are entered, previously specified points or text will be deleted).

2. Pen number.

3. Symbol number (if none is given, only text will be output).

4. Text (e.g., a legend; 0-25 characters).

5. Y-axis dataset (this specifies the dataset selected for a single histogram (actually the X-axis in this case), or for any dataset on a stacked plot of datasets).
   or
   Group number (this specifies the group for a stacked plot of groups for one dataset).

Note that the given XY co-ordinates define the centre of the symbol or, if no symbol is specified, the bottom of the first character of text. The maximum number of added points and/or text lines is 20. All those required for a given plot (either single or stacked) must be specified in one operation).

(15) List statistics (for all samples in the selected groups and for selected datasets; may be printed from file GDA.PRN).

(9) Display XY Plot

As for datasets and histograms, plots may be single or stacked. Menu items 1-12 are identical to the display dataset menu. The remainder are as follows:

(13) Define pen for least-squares line (1 of up to 8 colours; displays least-squares line for all groups selected for display in 15; if log axes are selected, line will be calculated on the log values).

(14) Define pen for regression polygons (different colours may be specified for 1st, 2nd and 3rd order regressions, calculated for all selected groups, using either values or log values).

(15) Select groups to be displayed.

(16) Specify additional plot points and/or text (additional points or text, such as a legend, may be added to previously selected plots via the keyboard:

1. X, Y co-ordinates (separated by a comma; previously specified points or text will be deleted if no values are entered here).

2. Pen number.
3. Symbol number (if none is given, only text will be output).
4. Text (e.g., sample number or a legend; 0-25 characters).
5. Y-axis dataset (this must be specified for each extra point or text required; for stacked plots, points or text may be added to any plot by specifying the appropriate dataset).

Note that the given XY co-ordinates define the centre of the symbols or, if no symbol is specified, the bottom of the first character of the text. If a new X-axis dataset is selected the added points may still appear, so be sure to delete any additional points (by choosing option 16 again, but not entering any XY co-ordinates) before selecting new datasets for display. All added points or text required for a given plot (either single or stacked) must be specified in one operation; the maximum number of added points and/or text lines is 20).

(17) Specify graphics overlay files (lines and/or text may be added by selecting an appropriate file - see appendix D for details of format and available files; make sure that the X and Y datasets are correct and the axis extremes are appropriate; the Y-axis dataset and name of the graphics overlay file (????.GRF) must be given).

(18) Regression curves for individual groups (as 14, except that curves are calculated separately for each displayed group).

(19) Least-squares lines for individual groups.

(20) List statistics (comprises minimum, maximum, mean, median, standard deviation, skewness, kurtosis, correlation coefficient, and 1st, 2nd and 3rd order regression coefficients, standard deviations, and T-values; calculated for all samples in the selected groups and for selected datasets or pairs of datasets (X with each Y); if log axes are selected for any dataset(s), statistics will be calculated using the natural logarithms of those dataset values; if regression curves for individual groups

are specified (18), statistics for each selected group will also be listed; results may be printed from file GDA.PRN).

An example of the statistics printout is given below.

SiO2

Minimum:	43.8000
Maximum:	77.4000
Mean:	66.7363
Median	69.4000
Standard Deviation:	7.7144
Skewness:	-1.1008
Kurtosis:	.4678

MgO

Minimum:	.0500
Maximum:	8.2800
Mean:	1.6046
Median	1.0200
Standard Deviation:	1.3806
Skewness:	1.9083
Kurtosis:	5.4701

Regression Statistics:

Independent Variable: SiO2
Dependent Variable: MgO

Correlation Coefficient: -.8217
Product-Moment Correlation Coefficient based on 80 pairs of values:
-.8217

Polynomial of degree 1	Standard error:	.79	
Regression Coefficient(s):	11.42	-.1470	
Coefficient(s) Standard Deviation:	.1155E-01		
T-Value(s):	-12.73		
Polynomial of degree 2	Standard error:	.79	
Regression Coefficient(s):	15.29	-.2735	.1011E-02
Coefficient(s) Standard Deviation:	.1690	.1348E-02	
T-Value(s):	-1.619	.7500	
Polynomial of degree 3	Standard error:	.78	
Regression Coefficient(s):	-45.87	2.798	-.4962E-01 .2746E-03
Coefficient(s) Standard Deviation:	1.624	.2667E-01	.1444E-03
T-Value(s):	1.723	-1.861	1.901

(10) Display Triangular Plot

Any 3 datasets may be selected for display on a triangular plot. File STDSET.DEF contains a number of sets of expressions for producing standard triangular diagrams (igneous AFM and ACF, Ti-Zr-Y, Ti-Mn-P, Nb-Zr-Y, and metamorphic A'KF, ACF, A'FM, SFA', and AFM). The menu is:

(1) Display (on screen or metafile 1-99).

(2) Select datasets (e.g., elements) for display.

(3) Change plot title (previous title is deleted if nothing is entered).

(4) Change apex titles.

(5) Display sample numbers.

(6) Select groups to be displayed.

(7) Specify additional plot points and/or text (additional plot points or text, such as a legend, may be added to previously selected plots via the keyboard; the following must be given:

1. X,Y,Z co-ordinates (separated by commas; either straight element concentrations or normalised co-ordinates (i.e., totalling to 100) may be used; previously specified points or text will be deleted if no values are entered here; co-ordinates outside the plotting ares (i.e., negative) are permissible, but obviously must be adjacent to the plot).

2. Pen number.

3. Symbol number (if none is given, only text will be output).

4. Text (e.g., sample number or a legend; 0-25 characters).

Note that the given XYZ co-ordinates define the centre of the symbol or, if no symbol is specified, the bottom of the first character of text. All added points or text required for a given plot must be specified in one operation; the maximum number of added points and/or text lines is 20. To align 2 or more lines of text vertically - for each unit decrease in the Y co-ordinate, increase X and Z by 0.5 each).

(8) Specify graphics overlay file (give file name).

(11) Display spidergram

Three basic types of spidergram may be plotted - single spidergrams for all selected groups, stacked spidergrams for each selected group, and single spidergrams for one or more samples identified by sample number. The standard spidergram utilises the default file (SPIDER.DEF), but other files are available for other types of spidergram (e.g., ARACH.DEF, REE.DEF, SPIMOD.DEF, see Appendix C). Other files may be written, using the same format if different elements and/or normalising values are required. It is also possible to normalise each group of samples against another in the file (not necessarily in the displayed groups) selected by its sample number. The menu is as follows:

(1) Display (on screen or as metafile 1-99; the default file is SPIDER.DEF, but another may be specified; if a normalising sample number is entered, the selected groups are normalised to that and an alternative Y-axis title may be specified; the default linetype is 1, but others may be specified in the 'define main plot parameters' option of the GDA starting menu).

(2) Change plot title.

(3) Display sample numbers.

(4) Set axes extremes to data range plus 20% (this is the default option, values for all groups (not just those selected for display) being used when setting limits).

(5) Set axes extremes to nice limits (powers of 10).

(6) Set axes extremes to typed-in values.

(7) Select groups to be displayed.

(8) Select spidergram type.

1. Single spidergram (for all selected groups).
2. Stacked for groups (each selected group displayed separately, with group numbers at right).
3. Single spidergram for typed-in sample numbers.

(9) Specify additional plot points and/or text (for spidergrams, this option is mainly useful for adding text, such as a legend, to a previously selected plot:

1. X,Y co-ordinates (separated by a comma; the X co-ordinate is defined by the number of elements on the axis (e.g., for a standard spidergram with 16 elements, the length of the X-axis is 17 units), and the Y-axis co-ordinate is the actual value; if no values are entered, previously specified points or text will be deleted).

2. Pen number.

3. Symbol number (if none is given, only text will be output).

4. Text (e.g., a legend; 0-25 characters).

5. Group number (specifies the group for a stacked plot of individual groups only).

Note that the given XY co-ordinates define the centre of the symbol or, if no symbol is specified, the bottom of the first character of the text. All added points or text required for a given plot (either single or stacked) must be specified in one operation; the maximum number of added points and/or text lines is 20).

(10) Display symbols on spidergram (if symbols are not nominated for display, only the lines are plotted).

(12) Display Legend

This may be used to display the symbols and pen colours assigned to sample groups. It may be written to a metafile so that the legend may be output to a plotter (Figure 1).

5.4 CIPW NORMS AND OTHER FACILITIES

Item 5 on the GDA menu allows all plotfiles to be deleted and item 14 allows a different GDA file to be specified (you will need to extract new datasets and reselect groups for display). Item 13 permits CIPW norms (weight percent) to be printed for all assigned samples, or for a specified range of samples (in GDA file order); in either case, samples from all groups or a single selected group may be printed. Alternatively, analyses may be entered from the keyboard by choosing this option after specifying the CIPW norm parameters. Examples of the CIPW norm printout (from file GDA.PRN) are given below. The first comprises samples on a GDA file (actually averages calculated in the UTIL program). The second is for data entered from the keyboard. Normative 'diopside' compositions are expressed in terms of the two endmembers diopside (Di, $CaMgSi_2O_6$) and hedenbergite (Hd, $CaFeSi_2O_6$). If required, they may be recalculated in terms of the three pyroxene endmembers as follows: enstatite (En, $Mg_2Si_2O_6$ = 0.464Di), ferrosilite (Fs, $Fe_2Si_2O_6$ = 0.532Hd), and wollastonite (Wo, $Ca_2Si_2O_6$ = 0.536Di + 0.468Hd). Note that in this program Cr (as Cr_2O_3) is treated as a major element, normative chromite always being calculated. The program requires fields for all major (including H_2O, CO_2, and LOI) and relevant trace (Ba, Li, Rb, Sr, Zr, V, Cr, Ni, S, F and Cl) elements to be present, although dummy fields on the Oracle (ASCII) file header will be sufficient for elements for which there are no data. Alternatively, any missing fields can be added using the UTIL program.

CIPWN

CO2 EXCLUDED FROM THE CALCULATIONS

	all	1	2	3	4	5
SiO2	65.81	65.84	69.14	64.26	70.83	69.87
TiO2	.76	.74	.54	.64	.48	.69
Al2O3	15.71	15.07	14.90	15.31	14.23	13.72
Cr2O3	.01	.00	.00	.01	.01	.00
Fe2O3	.99	1.03	.70	1.57	.39	.89
FeO	4.67	3.71	2.88	4.55	3.14	3.07
MnO	.08	.08	.07	.08	.05	.05
MgO	1.87	1.62	1.13	2.39	1.14	.54
CaO	2.77	3.77	2.45	5.83	2.24	2.01
Na2O	2.43	3.38	3.01	2.68	2.51	2.22
K2O	3.72	3.53	4.26	1.76	4.06	5.78
P2O5	.14	.25	.11	.17	.11	.22
H2O+	.54	.43	.49	.33	.41	.59
TOTAL	99.49	99.45	99.68	99.57	99.59	99.65

NORMATIVE MINERAL COMPOSITION, CALCULATED USING METHOD OF KELSEY (1965)

	all	1	2	3	4	5
Quartz	26.06	20.96	26.90	24.28	32.39	28.59
Corundum	2.98	.00	1.13	.00	1.91	.68
Orthoclase	22.01	20.89	25.19	10.41	23.97	34.16
Albite	20.60	28.60	25.46	22.64	21.20	18.79
Anorthite	12.81	15.50	11.48	24.55	10.37	8.53
Diopside	.00	1.34	.00	2.74	.00	.00
Diopside (CaMg)	.00	.65	.00	1.44	.00	.00
Hedenbergite	.00	.69	.00	1.30	.00	.00
Hypersthene	11.28	8.26	6.74	10.73	7.60	5.21
Enstatite	4.65	3.73	2.81	5.27	2.85	1.36
Ferrosilite	6.64	4.54	3.93	5.45	4.76	3.86
Magnetite	1.43	1.49	1.02	2.27	.56	1.29
Chromite	.01	.00	.01	.01	.01	.00
Ilmenite	1.45	1.40	1.02	1.22	.90	1.31
Apatite	.33	.58	.25	.39	.27	.53

DERIVED VALUES FOR STANDARD EXPRESSIONS

	all	1	2	3	4	5
Diff. Index	68.67	70.45	77.54	57.33	77.56	81.53
Colour Index	14.17	12.50	8.79	16.96	9.07	7.81
Pl=Ab+An	33.40	44.10	36.94	47.20	31.57	27.31
100An/(Ab+An)	38.34	35.15	31.07	52.02	32.86	31.22
100An/(An+Ab^)	38.34	35.15	31.07	52.02	32.86	31.22
Ab^=Ab+1.85Ne	20.60	28.60	25.46	22.64	21.20	18.79
Q"=Q+0.3En+.23Fs	28.97	23.11	28.63	27.10	34.32	29.87
Ol^=Ol+.7En+.8Fs	8.38	6.11	5.01	7.91	5.67	3.93
Ne^=Ne+.54Ab	11.16	15.50	13.80	12.27	11.49	10.18
Q^=Q"+.46Ab	38.40	36.21	40.30	37.47	44.03	38.47
mg number	41.62	43.69	41.18	48.32	39.33	24.00

CIPWN

CO2 EXCLUDED FROM THE CALCULATIONS

	5603	5611	5640
SiO2	49.10	46.20	50.50
TiO2	2.47	.91	.51
Al2O3	9.87	11.75	17.46
Fe2O3	2.93	2.84	1.89
FeO	10.31	5.96	7.55
MnO	.19	.14	.18
MgO	12.57	13.49	8.30
CaO	8.94	7.62	11.00
Na2O	1.83	1.58	1.33
K2O	.90	4.30	.20
P2O5	.24	.70	.05
H2O+	.81	1.94	1.00
TOTAL	100.16	97.43	99.97

NORMATIVE MINERAL COMPOSITION, CALCULATED USING METHOD OF KELSEY (1965)

	5603	5611	5640
Quartz	.00	.00	3.67
Orthoclase	5.32	25.41	1.18
Albite	15.48	6.25	11.25
Anorthite	16.06	12.27	41.08
Nepheline	.00	3.86	.00
Diopside	21.52	16.65	10.70
Diopside (CaMg)	15.87	13.99	7.14
Hedenbergite	5.65	2.67	3.55
Hypersthene	25.63	.00	27.26
Enstatite	18.20	.00	17.36
Ferrosilite	7.43	.00	9.90
Olivine	5.84	23.58	.00
Forsterite	4.03	19.00	.00
Fayalite	1.81	4.58	.00
Magnetite	4.25	4.12	2.74
Ilmenite	4.69	1.73	.97
Apatite	.57	1.66	.12

DERIVED VALUES FOR STANDARD EXPRESSIONS

	5603	5611	5640
Diff. Index	20.80	31.66	16.10
Colour Index	61.93	46.08	41.67
Pl=Ab+An	31.54	18.52	52.33
100An/(Ab+An)	50.91	66.26	78.50
100An/(An+Ab^)	50.91	47.85	78.50
Ab^=Ab+1.85Ne	15.48	13.37	11.25
Q"=Q+0.3En+.23Fs	7.14	.00	11.12
Ol^=Ol+.7En+.8Fs	24.34	23.58	19.81
Ne^=Ne+.54Ab	8.39	7.24	6.10
Q^=Q"+.46Ab	14.23	2.86	16.27
mg number	68.48	80.13	66.20

5.5 PLOT TYPES

Examples of the various types of plot which can be produced are shown on the following pages.

Figure 5 shows the basic plot types available. All were output to a Graphtec plotter at four per page, using the default axis lengths (25 x 20 cm, except figure 5E), and symbol, tick, and axis label sizes. They are shown at actual size, i.e., all XY plots, except Figure 5E are 12.5 x 10 cm. Figure 5A is a dataset display of MgO for six sample groups.

Figures 5B-D show the three types of histogram. Figure 5B includes histograms of three elements for all samples; 5C shows separate histograms of TiO2 for each of four sample groups (1-4); and 5D is a single histogram of SiO2 for all samples.

Figures 5E-J are various XY plots. Figure 5G is a plot of ppm K against ppm Rb. K was selected as a typed-in expression (8301 * K20). This plot includes separate least-squares lines for each group (in the same colours as the corresponding group symbols on the original). Figure 5H (TiO2 against SiO2) shows mean lines and first, second, and third order regression lines for all groups combined. Figure 5I also shows regression lines; Ce/Y was selected as a typed-in expression. Figure 5E uses logarithmic axes. As both axes are three cycles (i,e., three orders of magnitude) long, the axes lengths were set to 20 x 20 cm to give a square final plot. Figure 5J is a stacked plot of three elements and an arithmetic expression (ASI, alumina saturation index). Note that the numbers of X-axis ticks and labels are much reduced.

Figures 5K-M are examples of spidergrams. Figures 5L and M used the default spidergram plot definition file SPIDER.DEF, whereas SPIMOD.DEF was used for Figure 5K. The latter shows three samples specified by their sample numbers, and each sample is plotted with different symbols and linetypes. Figure 5L shows a plot of one sample group, and Figure 5M shows two stacked groups (1 and 2). In the latter plot, each sample was normalised to a specified sample (number 81285399), and the symbols were omitted. The appropriate Group name has been added to each plot as additional text.

Figures 5N and O are triangular plots. The former (Q-Ab-Or) includes an added point (123) and text (i.e., a legend), as well as the graphics overlay file QABOR.GRF (based on the experimental data of Tuttle & Bowen (1958) - see Appendix D). Note that such added plot points and text must be specified in the same operation. The igneous AFM plot (Figure 5O) was selected from the standard dataset definition file STDSET.DEF, and includes the graphics overlay file AFM.GRF.

Figure 5P is an example of a stacked XY plot for a single group showing sample numbers. These would normally only be displayed on the screen to allow individual samples to be identified.

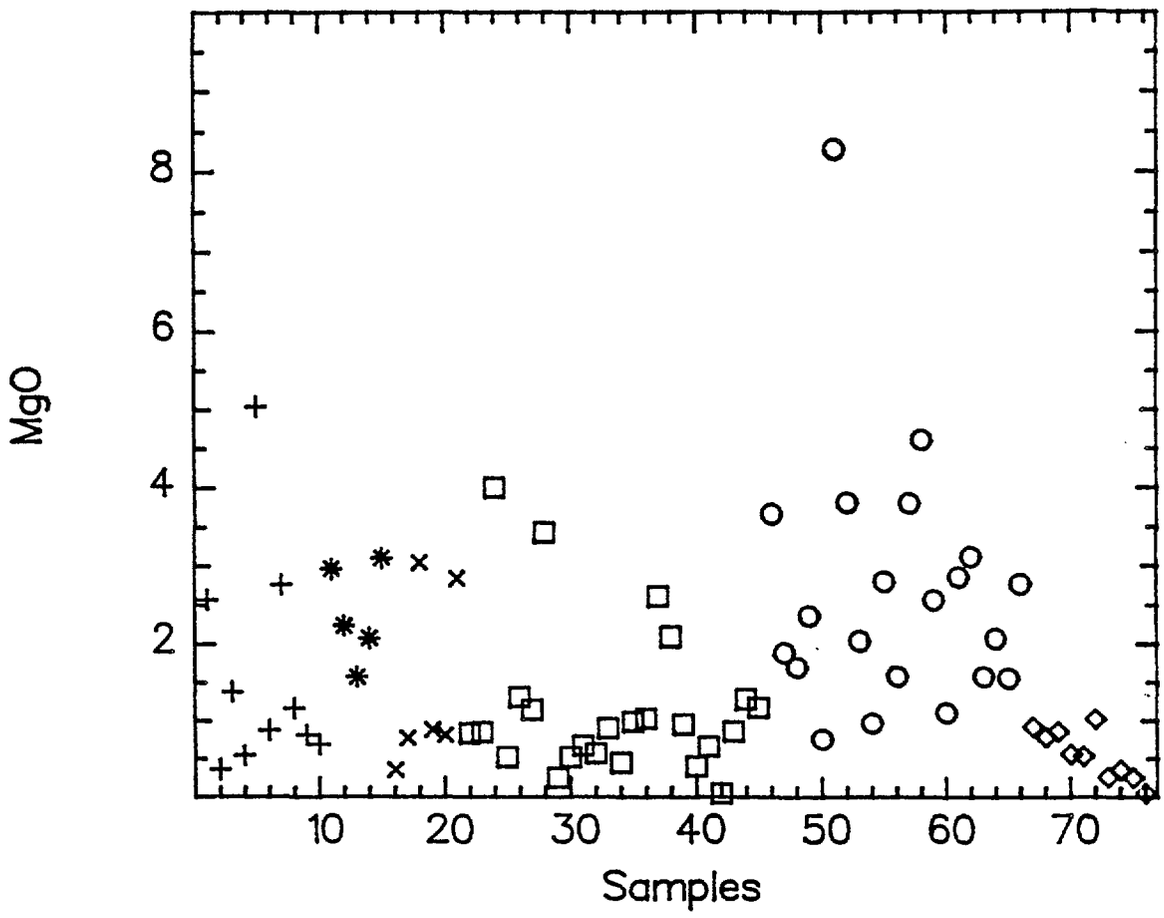

MgO
8
6
4
2
10
20
30
40
50
60
70
Samples

FIG. 5A

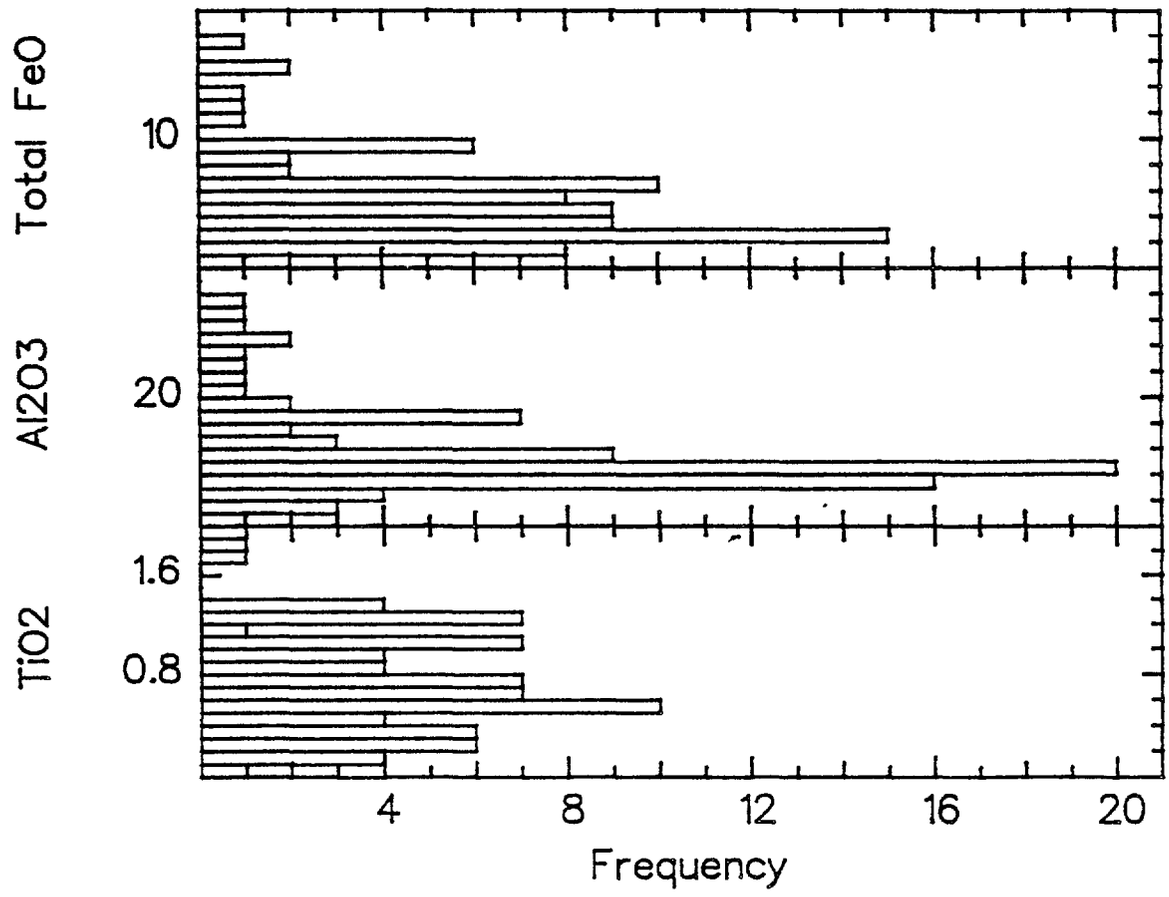

Total FeO
10
Al2O3
20
TiO2
1.6
0.8
4
8
12
16
20
Frequency

FIG. 5B

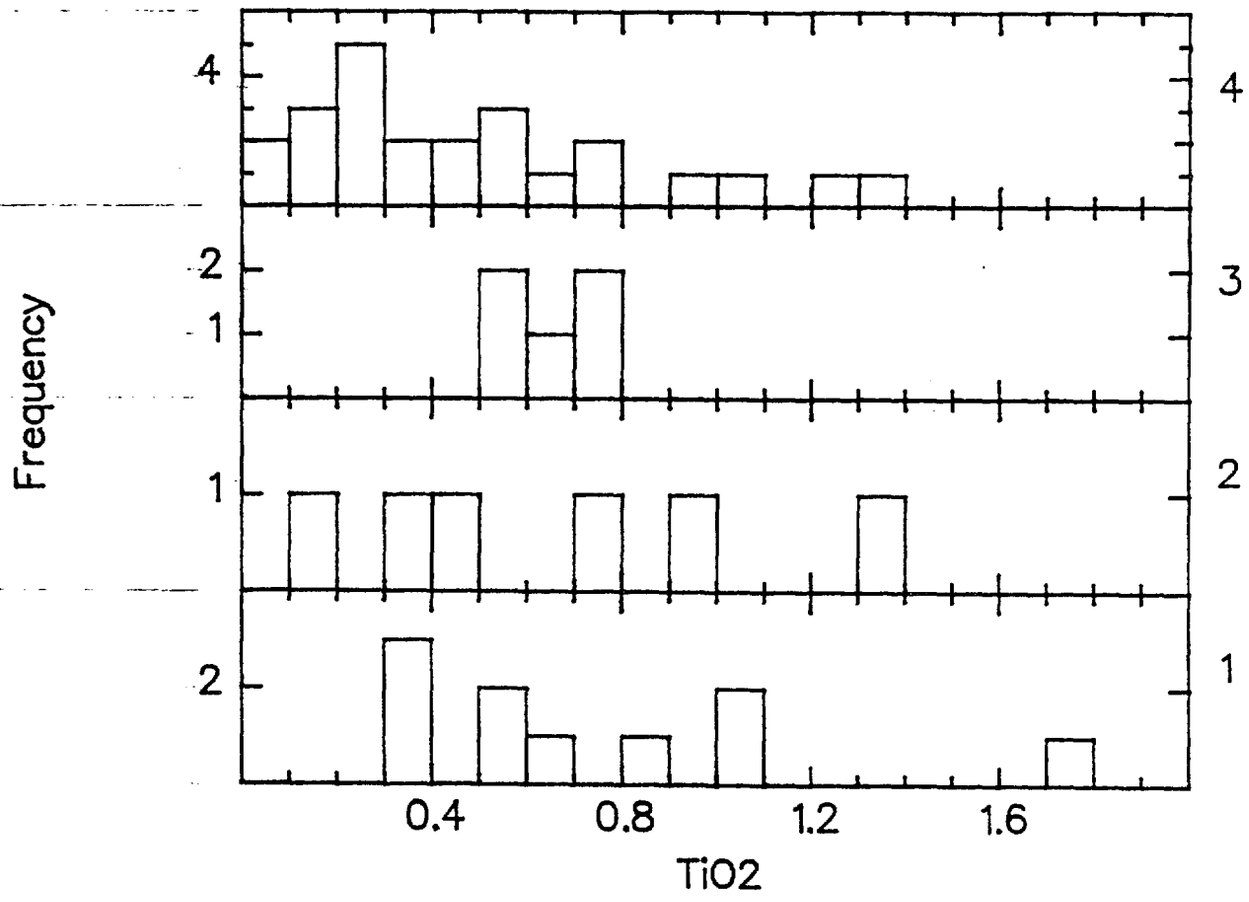

Frequency
4
2
1
1
2
4
3
2
1
0.4
0.8
1.2
1.6
TiO2

FIG. 5C

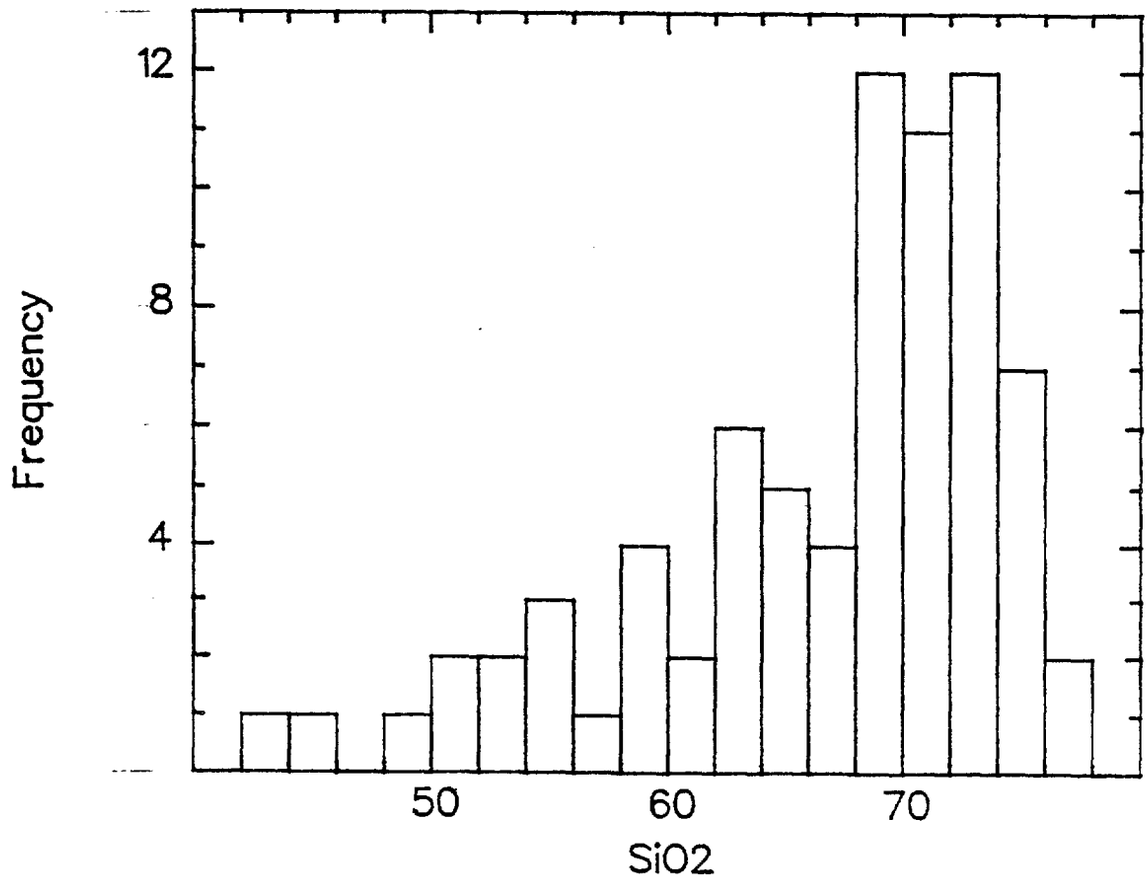

Frequency
12
8
4
50
60
70
SiO2

FIG. 5D

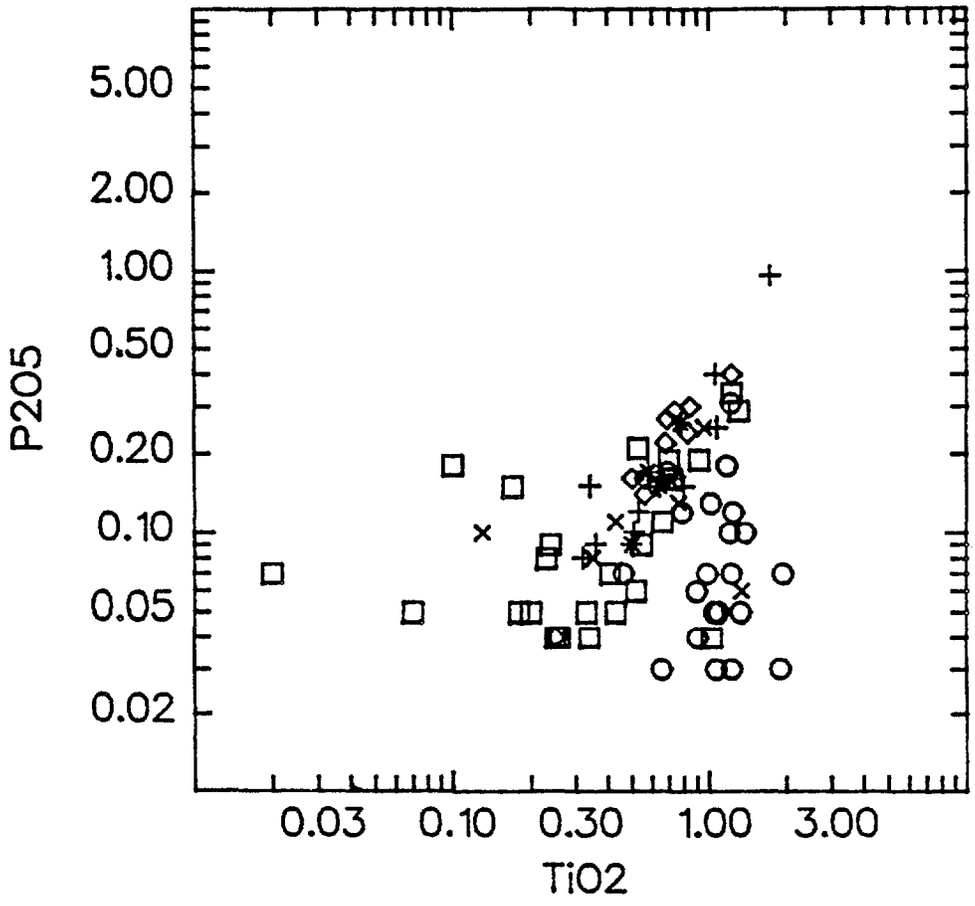

5.00
2.00
1.00
0.50
0.20
0.10
0.05
0.02
P205
0.03
0.10
0.30
1.00
3.00
TiO2

FIG. 5E

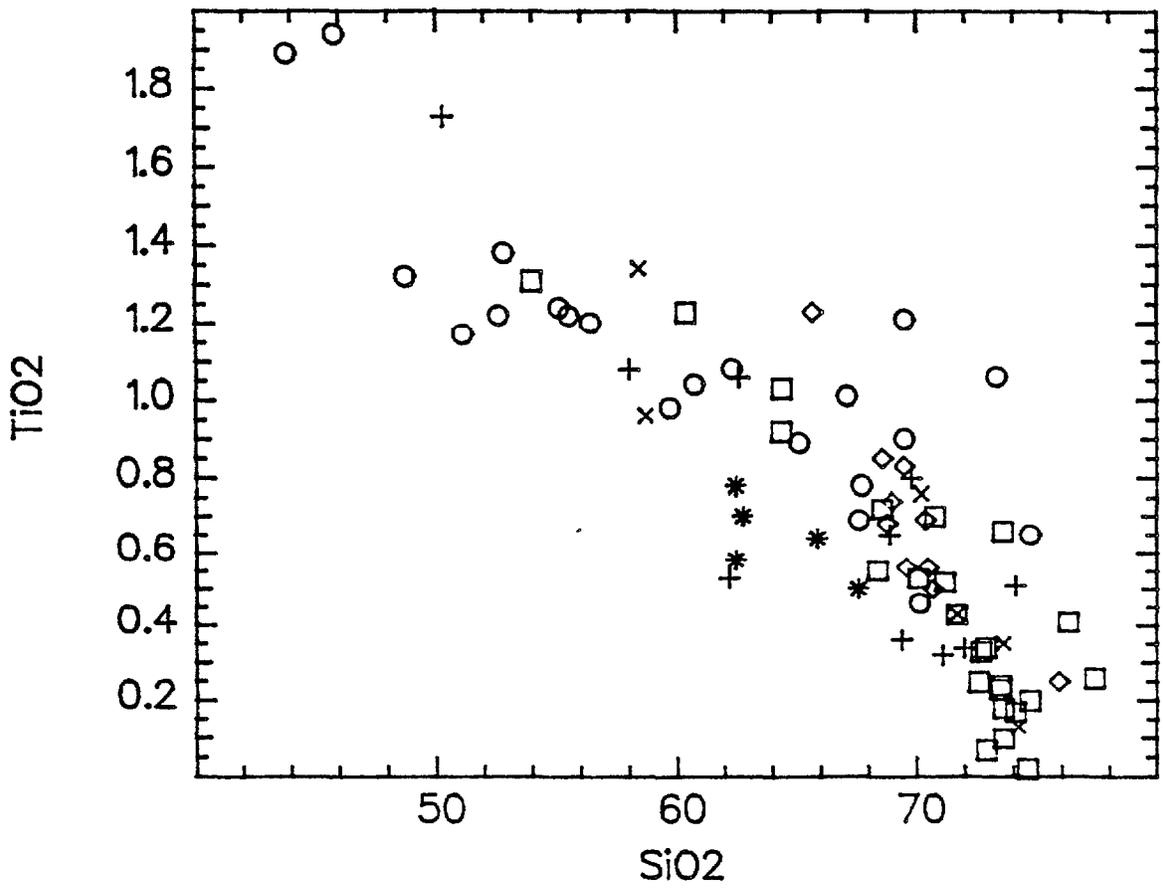

1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
TiO2
50
60
70
SiO2

FIG. 5F

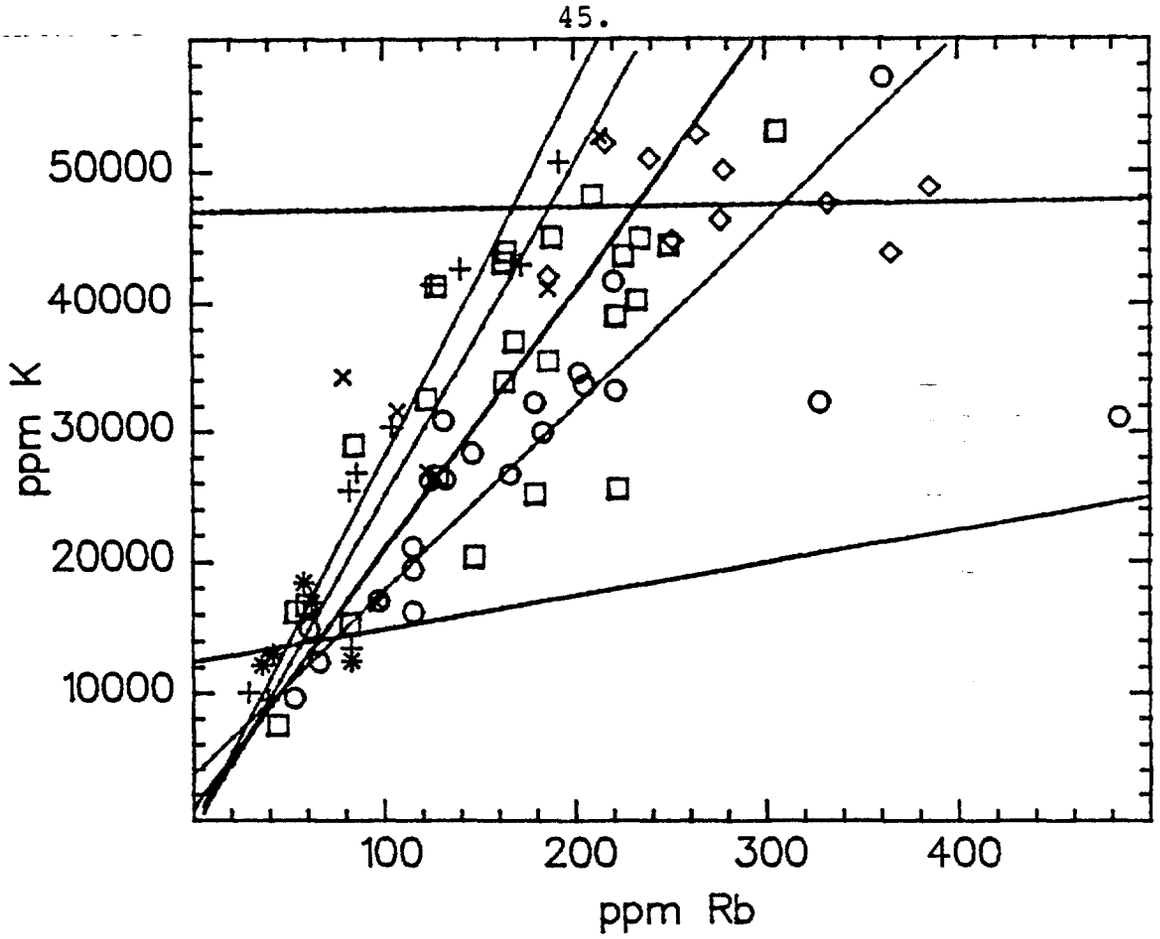

50000
40000
30000
20000
10000
ppm K
100
200
300
400
ppm Rb

FIG. 5G

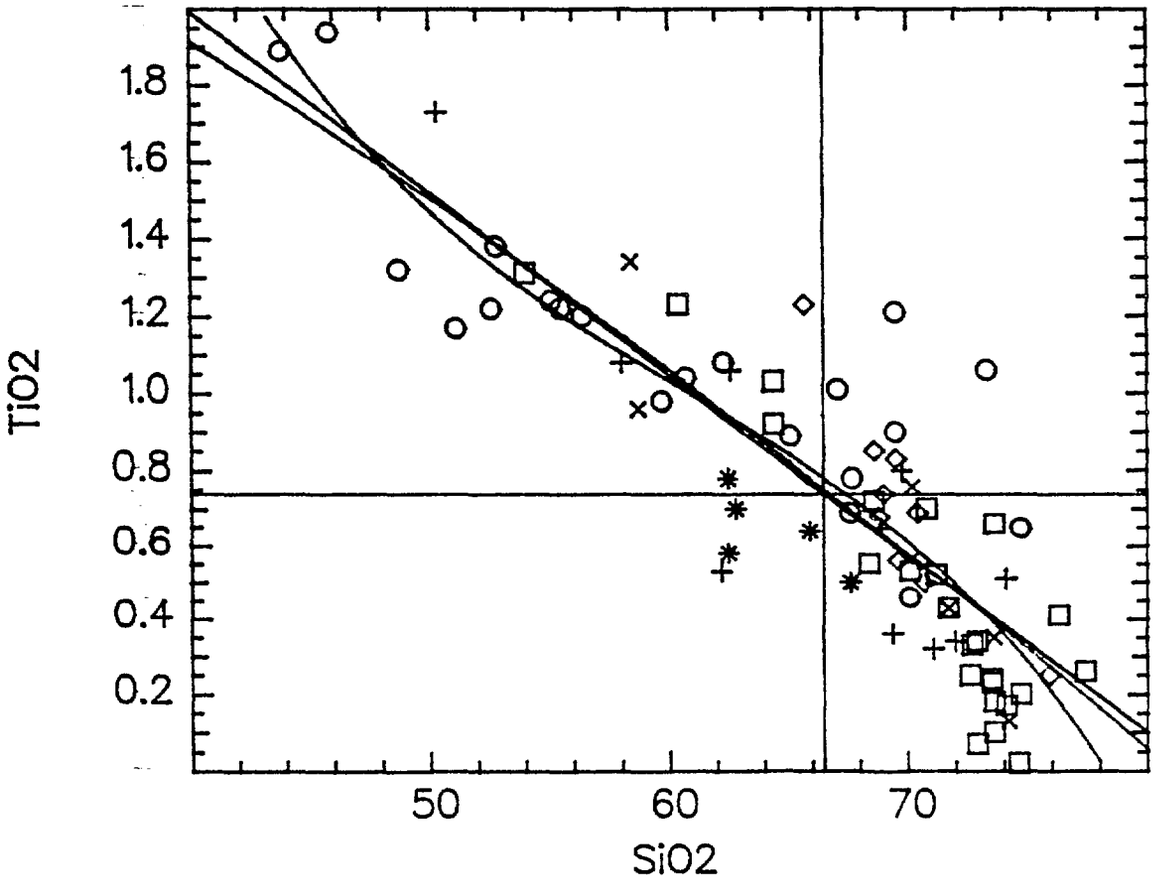

1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
TiO2
50
60
70
SiO2

FIG. 5H

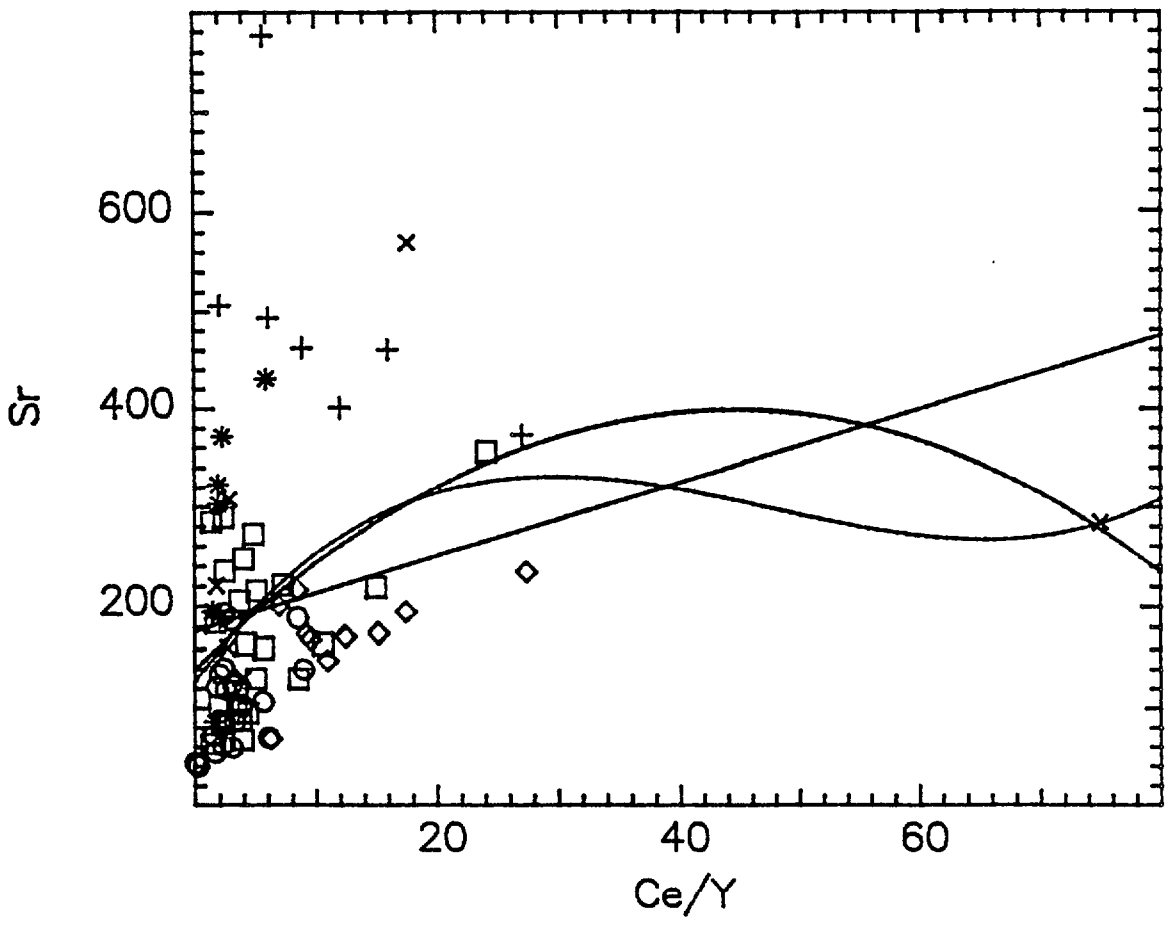

Sr
600
400
200
20
40
60
Ce/Y

FIG. 5I

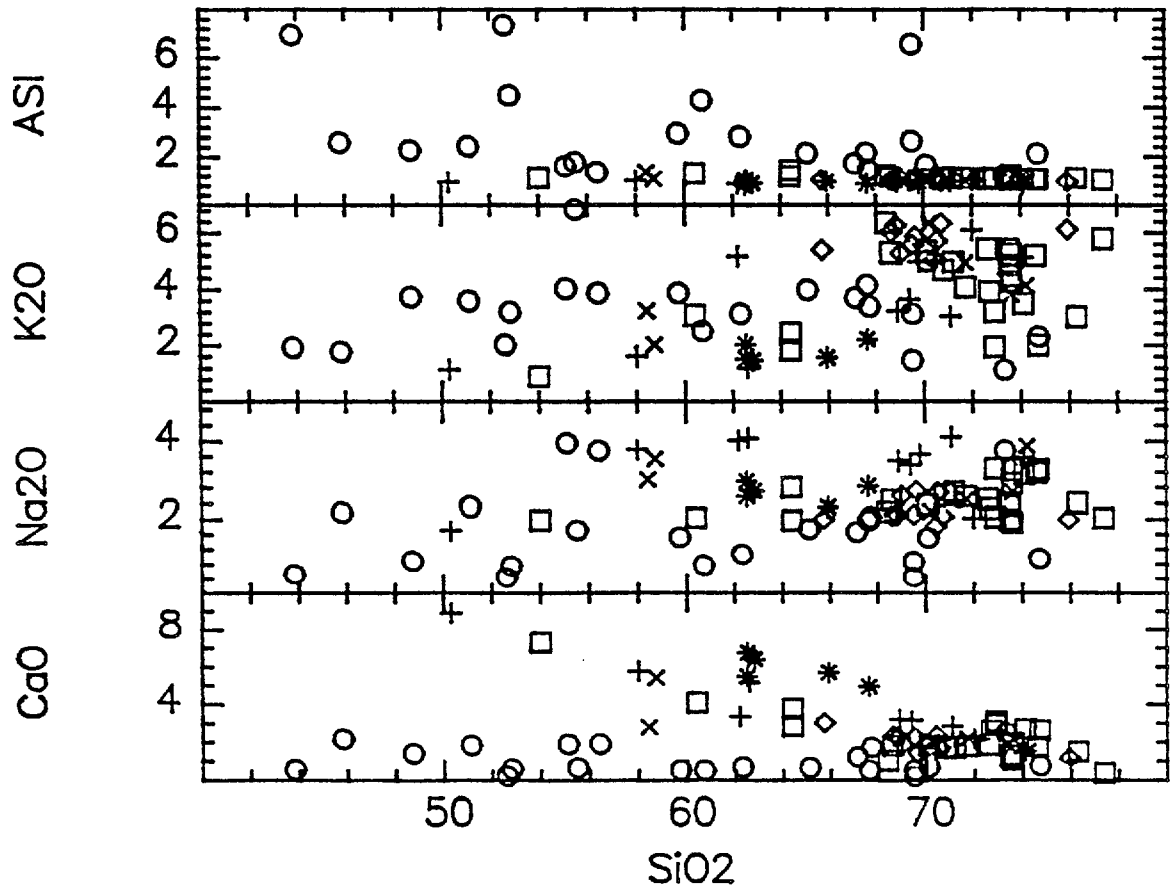

ASI
K2O
Na2O
CaO
6
4
2
6
4
2
4
2
8
4
50
60
70
SiO2

FIG. 5J

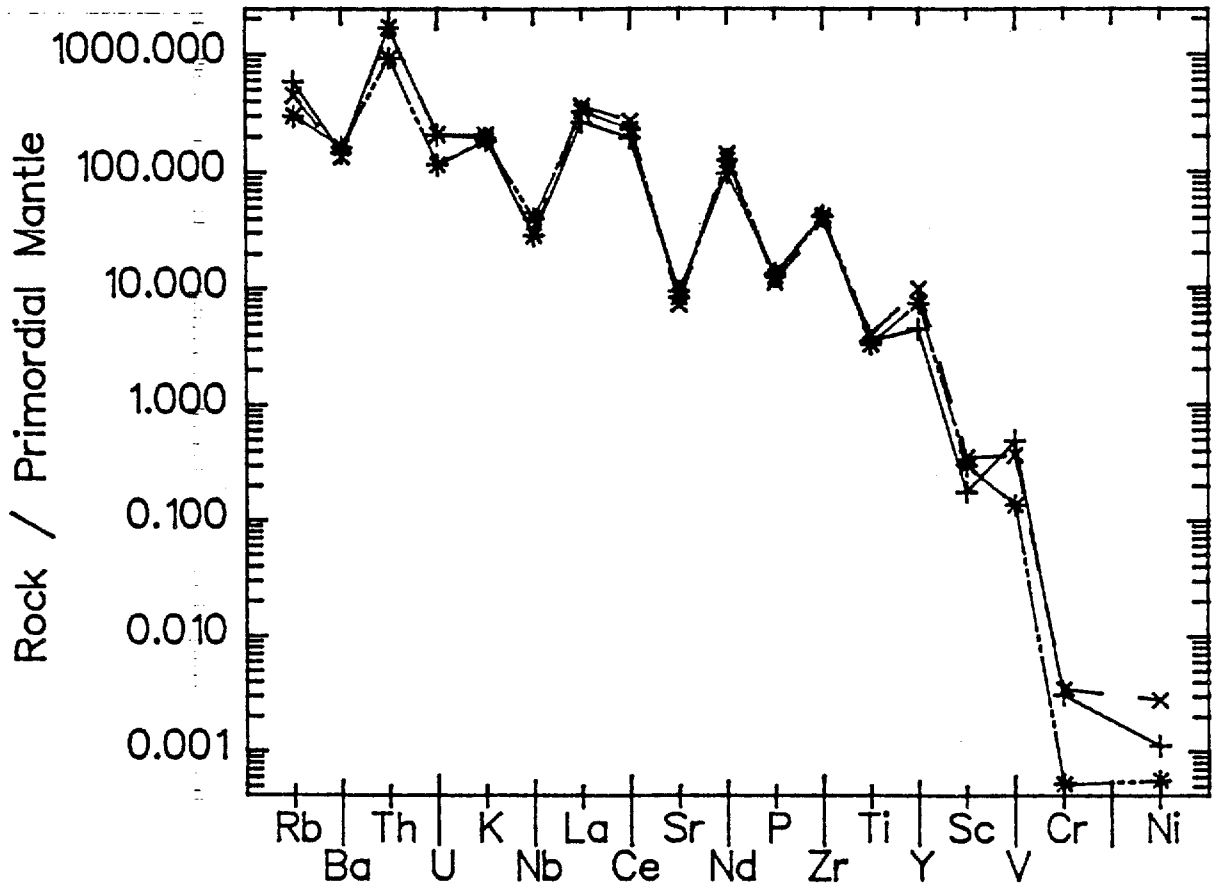

Rock / Primordial Mantle
1000.000
100.000
10.000
1.000
0.100
0.010
0.001
Rb
Ba
Th
U
K
Nb
La
Ce
Sr
Nd
P
Zr
Ti
Y
Sc
V
Cr
Ni

FIG. 5K

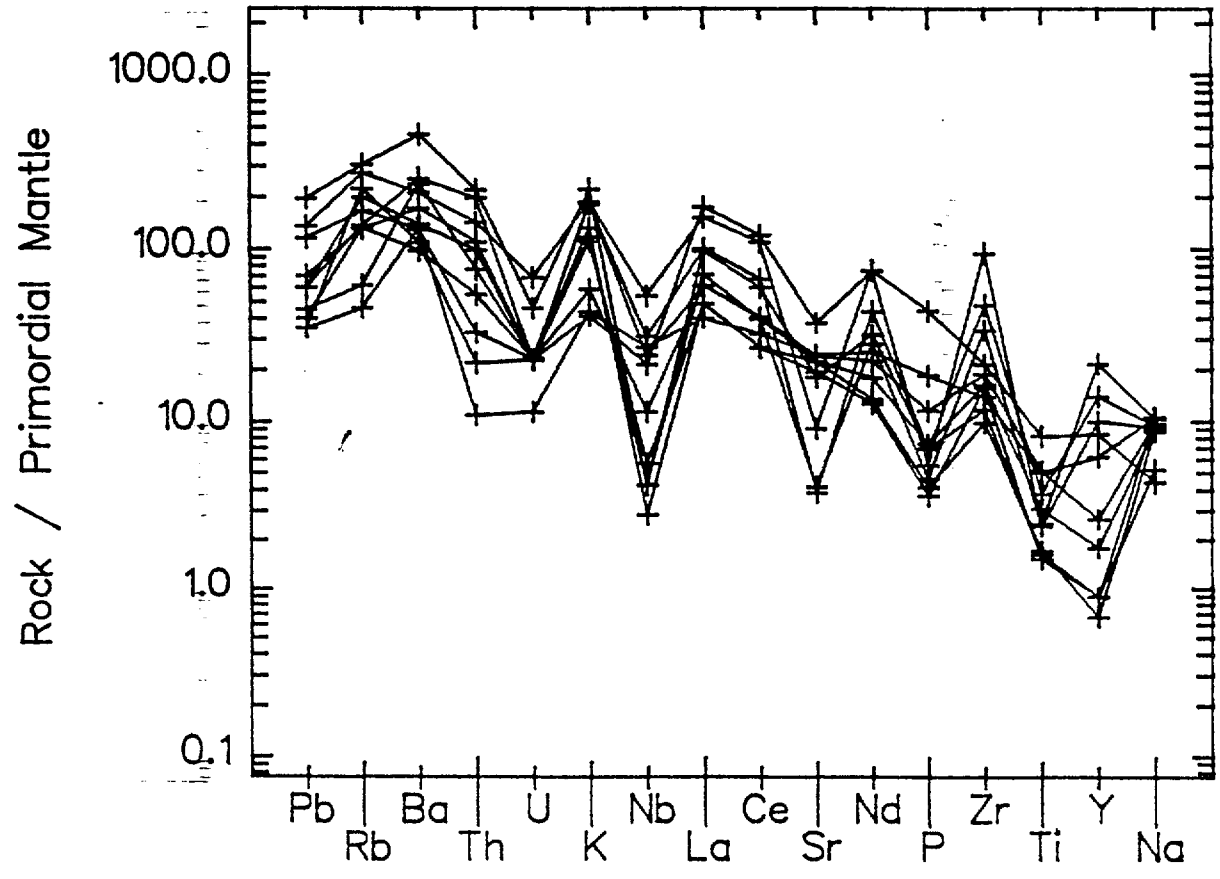

Rock / Primordial Mantle
1000.0
100.0
10.0
1.0
0.1
Pb
Rb
Ba
Th
U
K
Nb
La
Ce
Sr
Nd
P
Zr
Ti
Y
Na

FIG. 5L

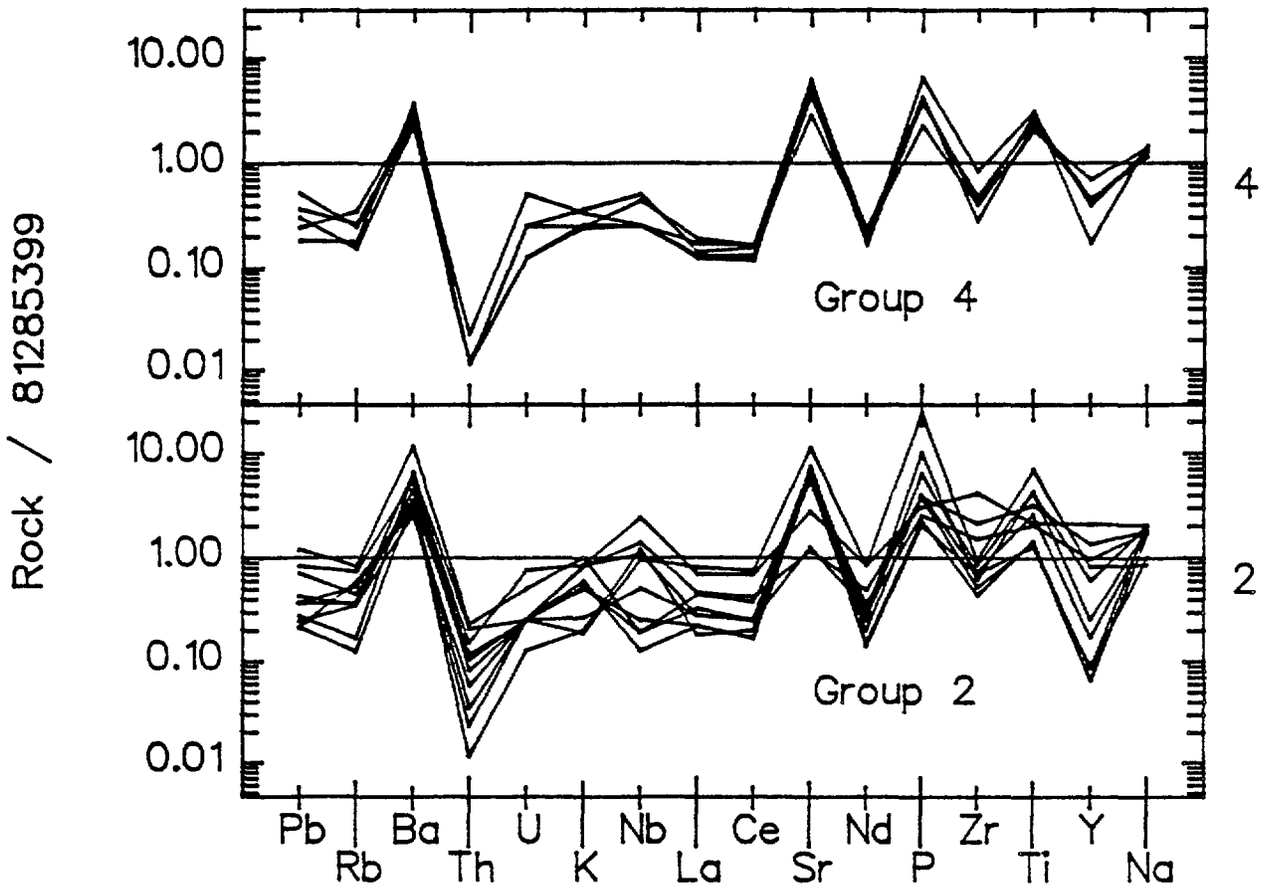

Rock / 81285399
10.00
1.00
0.10
0.01
Group 4
4
Group 2
2
Pb
Rb
Ba
Th
U
K
Nb
La
Ce
Sr
Nd
P
Zr
Ti
Y
Na

FIG. 5M

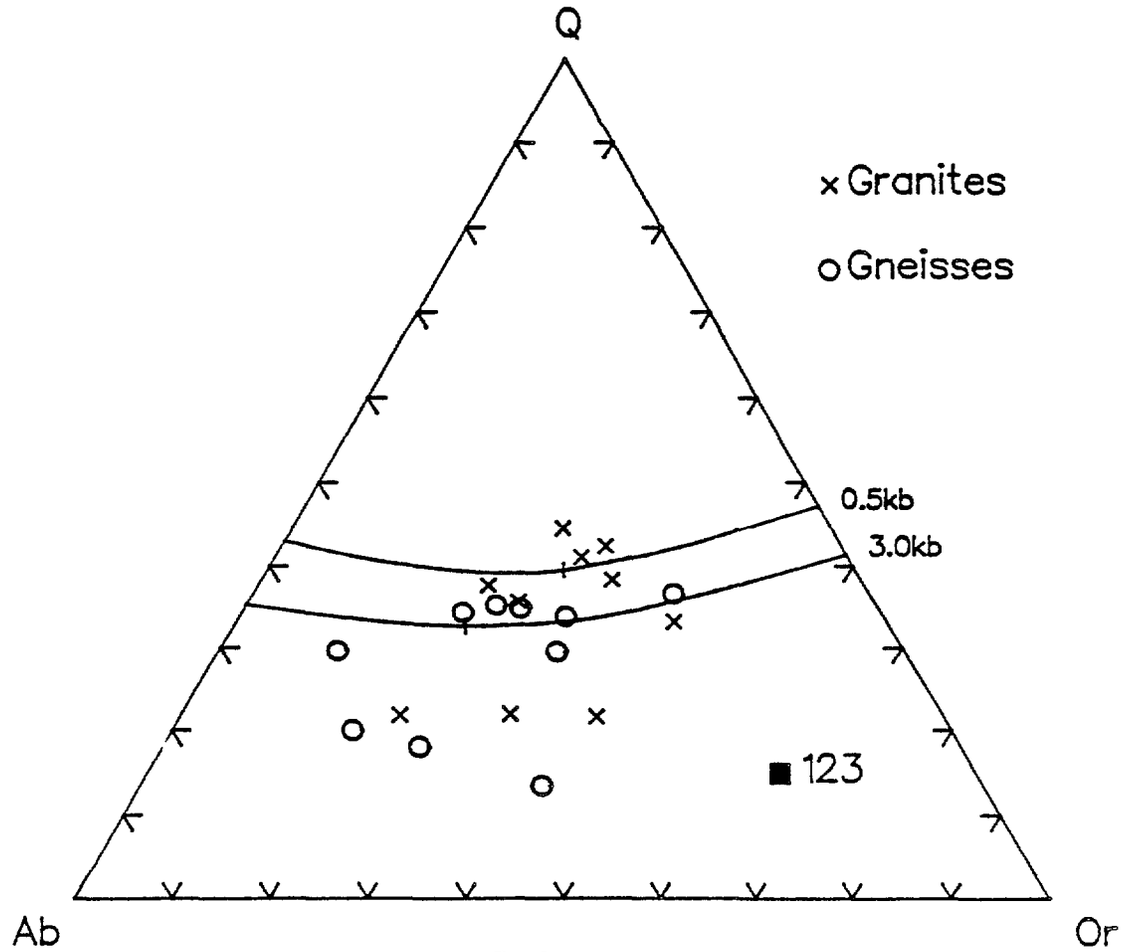

Q
× Granites
o Gneisses
0.5kb
3.0kb
■ 123
Ab
Or

FIG. 5N

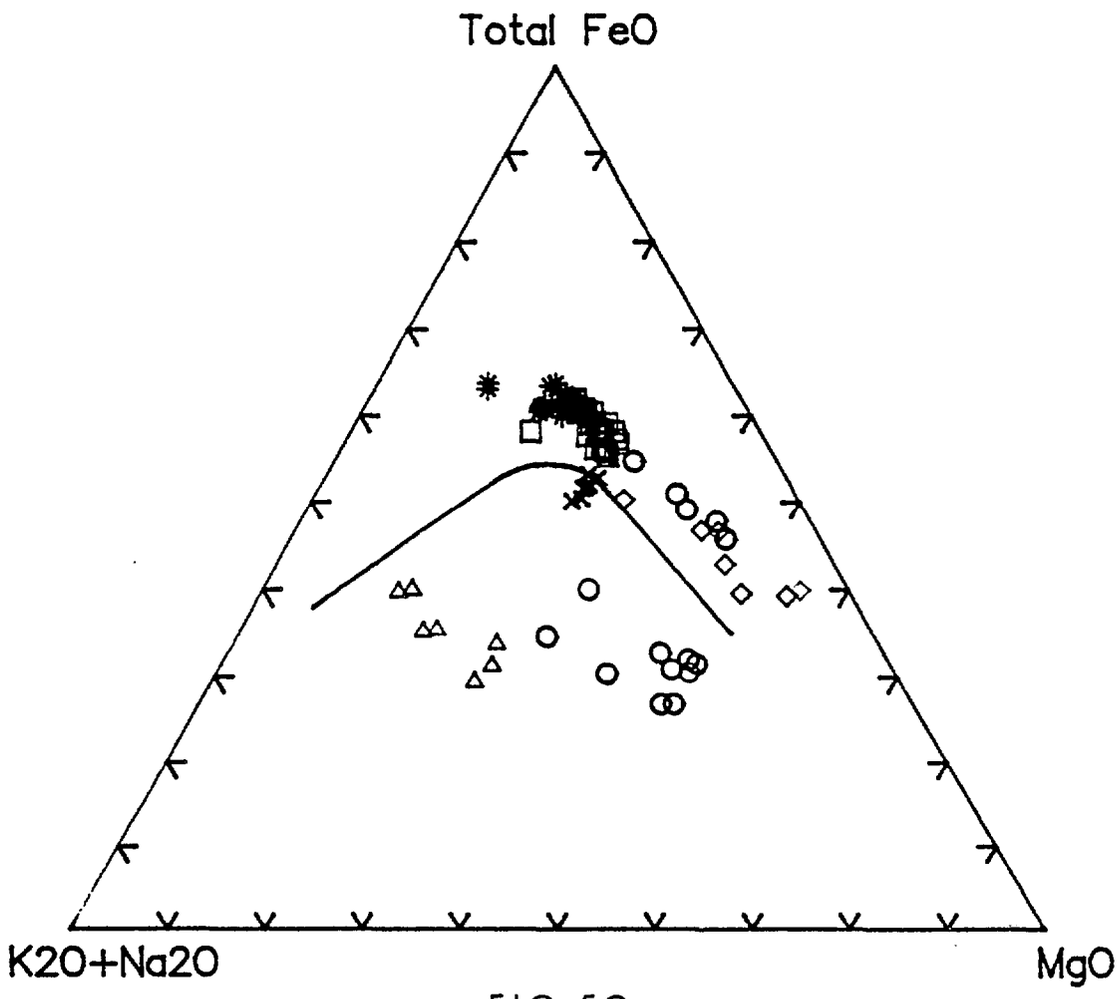

Igneous AFM (Weight %)
Total FeO
K2O+Na2O
MgO

FIG. 5O

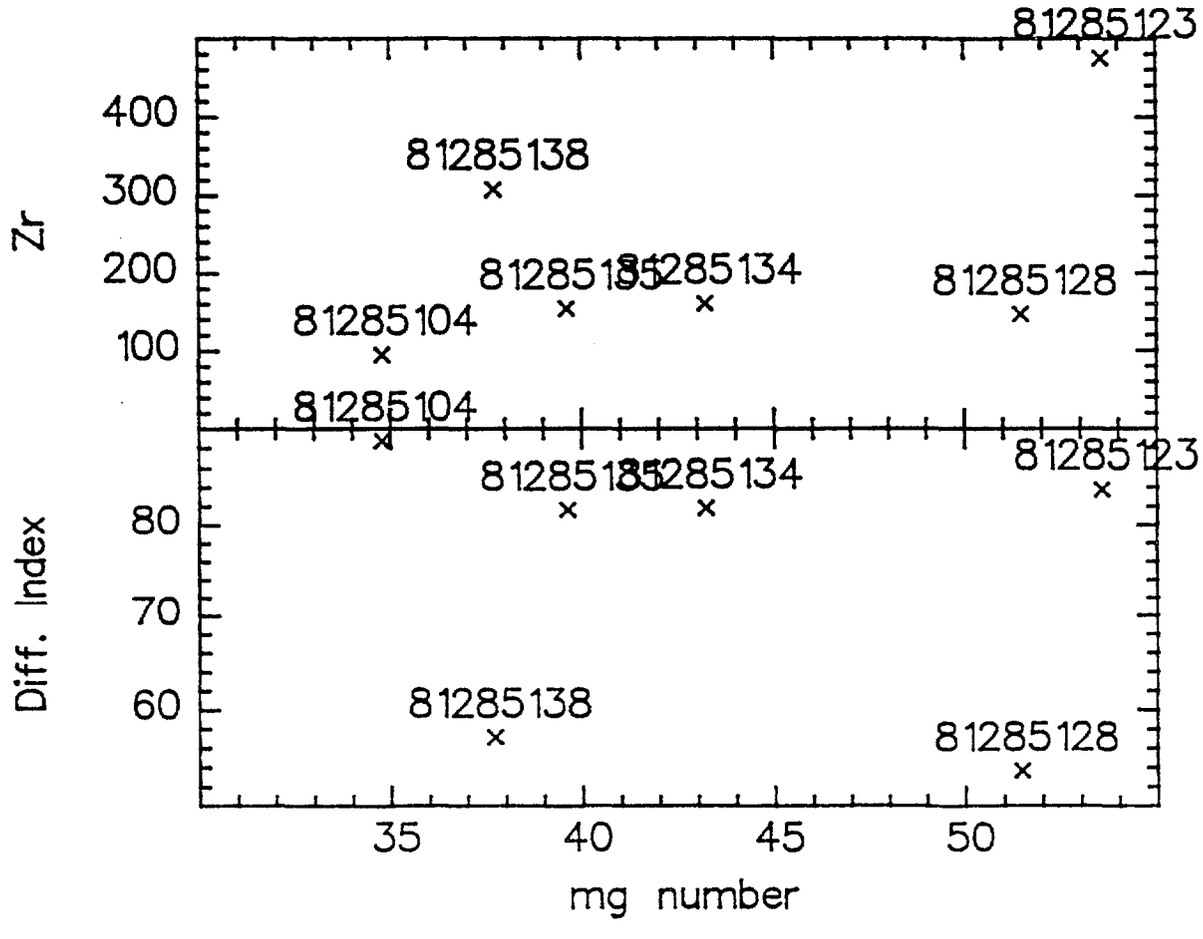

81285123
400
81285138
300
200
81285135
81285134
81285128
100
81285104
81285104
81285135
81285134
81285123
80
70
60
81285138
81285128
Zr
Diff. Index
35
40
45
50
mg number

FIG. 5P

Figure 6 shows three examples of stacked plots using different axis lengths to change the plot shape. All were plotted using the full Graphtec plotter page (i.e., one plot per page).

For Figure 6A, axis lengths (X, Y) were set to 12.5 x 20.0cm. Symbol size (0.3cm), tick size (0.5cm), and label size (0.6 cm) were all reduced.

Figures 6B and C are log - log plots, 2 x 1 and 3 x 1 elements, respectively. To produce the square plot shapes for each element pair (3 x 3 cycles), axis lengths were set to 10 x 20 cm for Figure 6B and 6.67 x 20 cm for Figure 6C. Symbol, tick, and label sizes were all set to half the default values (0.25, 0.5, and 0.5cm, respectively) in Figure 6B, and smaller (0.2, 0.35, 0.3cm, respectively) in Figure 6C. It is also possible to stack log-log plots with, for example, X = 3 cycles and each Y-axis element = 2 cycles, while still preserving the same scale for each axis. In this case axis lengths of 15 x 20 cms for a 2 x 1 element, and 10 x 20 cm for a 3 x 1 element plot would be appropriate. Of course, logarithmic scales do not have to be the same for each axis, but such plots are useful in studying variations in incompatible element ratios in tholeiite suites, for example. Lines of constant element ratio (Y/X) then have unit slope. However, it is not possible to do this if different Y-axis elements have different numbers of log cycles, as the Y axis is automatically divided into equal sections for each element. If this does happen, it is possible to change the axis extremes for any element. In fact, by judicious choice of both axis limits and axis lengths, any log-log plot, whether single or stacked, can be output with both axes having the same logarithmic scale.

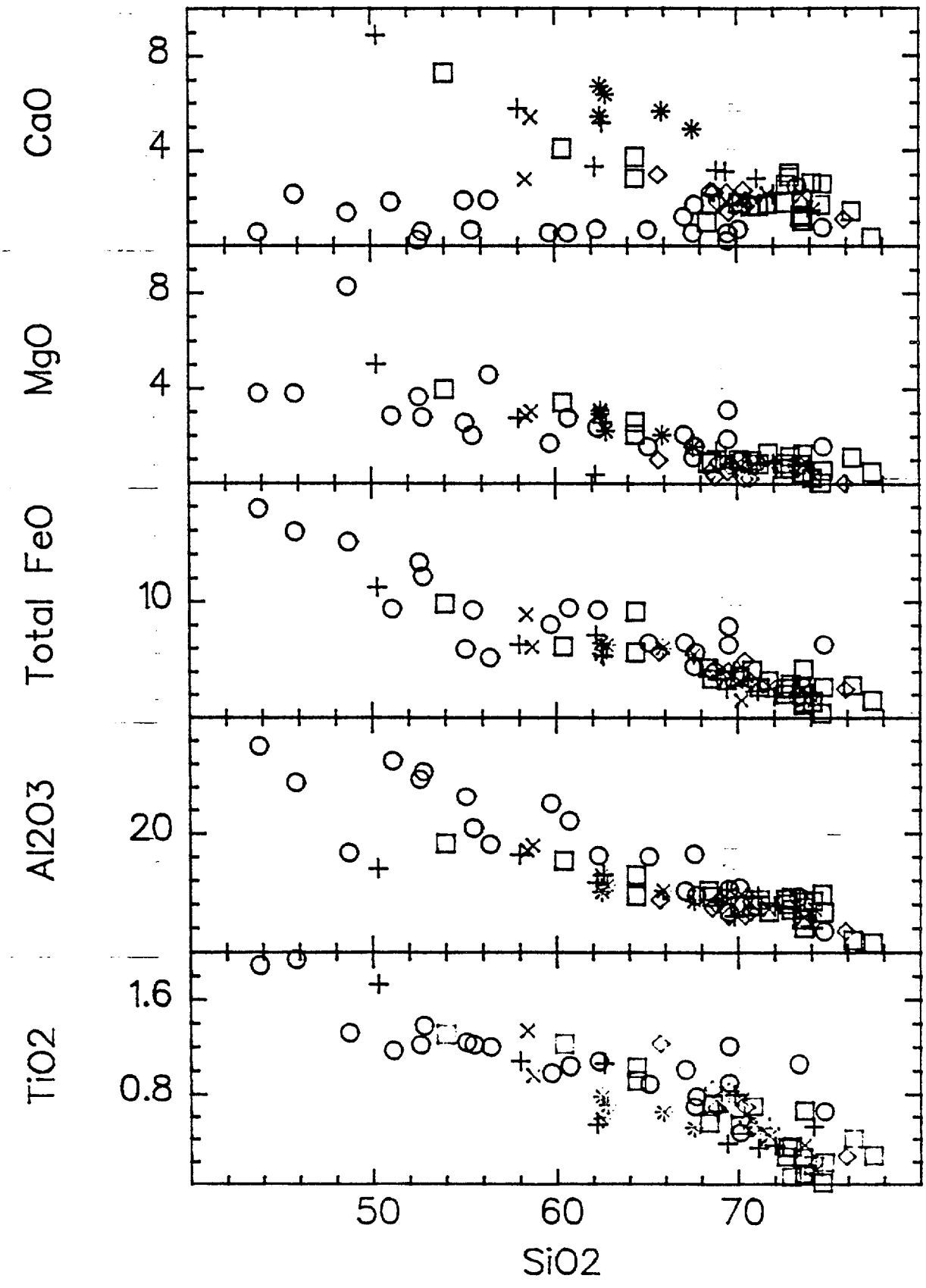


FIG. 6A

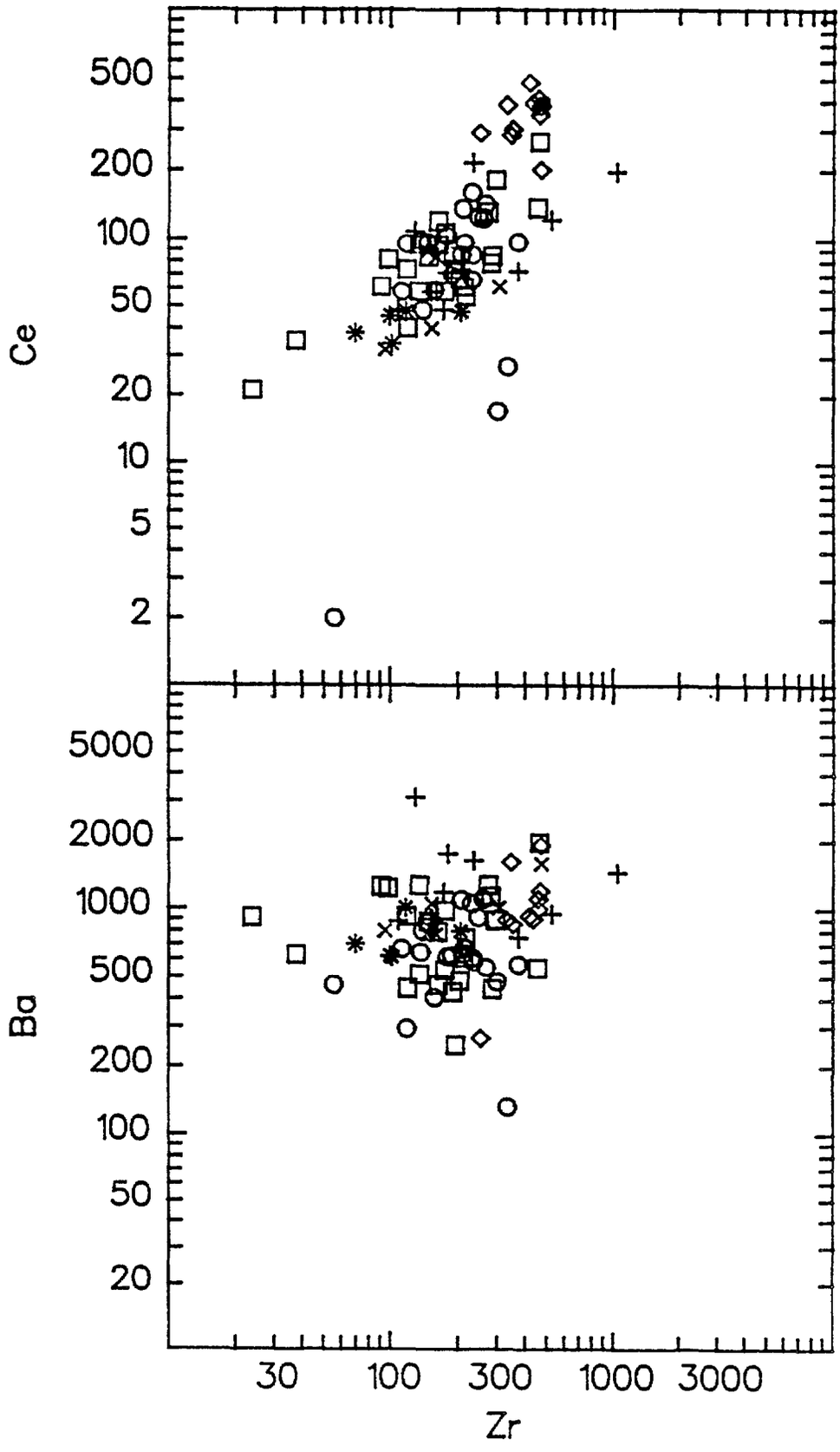

Ce
500
200
100
50
20
10
5
2
Ba
5000
2000
1000
500
200
100
50
20
30
100
300
1000
3000
Zr

FIG. 6B

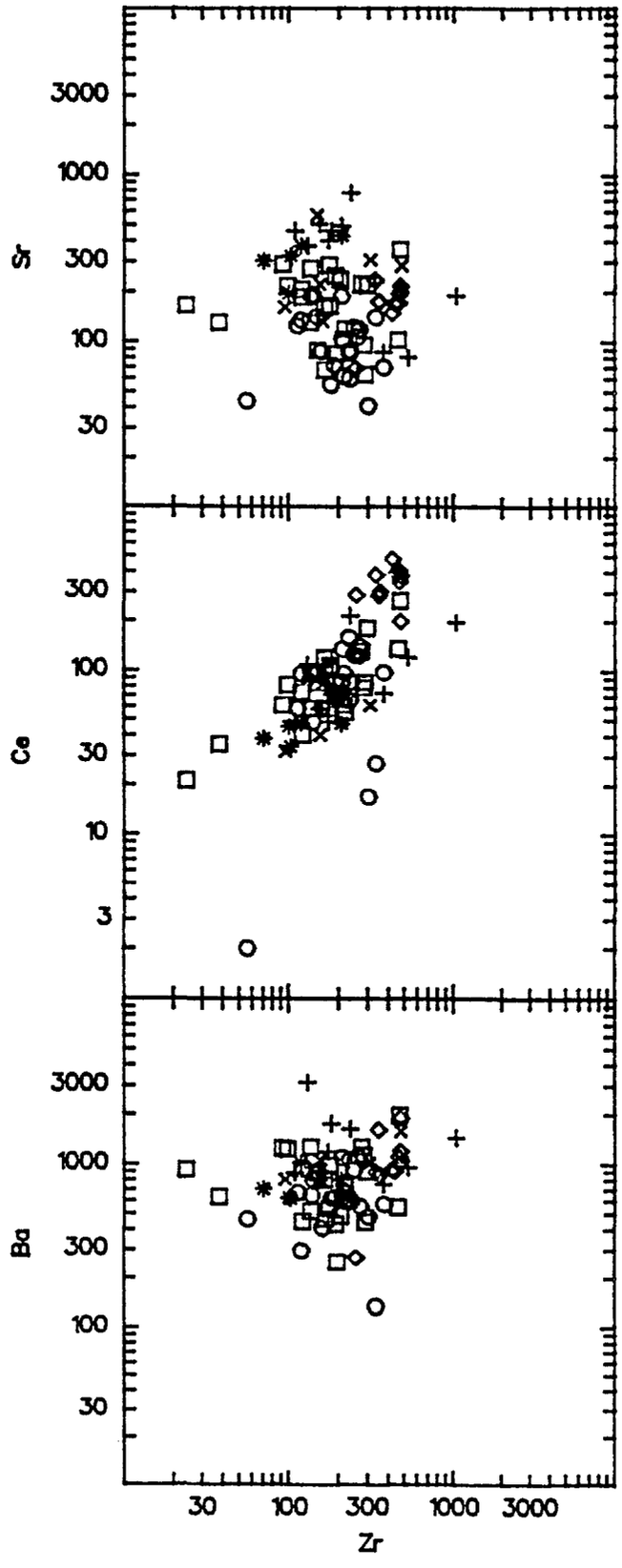

Sr
3000
1000
300
100
30
Ce
300
100
30
10
3
Ba
3000
1000
300
100
30
30
100
300
1000
3000
Zr

FIG. 6C

6. PLOT

Plots are generated as metafiles which are plotted by the HALO translator programs. Output to metafiles is carried out in the appropriate GDA plotting option (XY plot, triangular plot, etc). Metafiles can be output to a directly connected Hewlett-Packard (HP) or compatible (e.g., Graphtec) plotter using the PLOT program, or can be copied (metafile names are GDA1.PLT to GDA99.PLT) and transferred to a PC with a connected plotter. Alternatively, plots may be output to HPGL files via the PLOT program for use on other off-line HP plotters or laser printers. Such HPGL files will normally be named GDA1.HPG to GDA99.HPG.

Plots generated by the plotter are essentially as displayed on the screen, although white lines or text on the screen are plotted with a black pen, and the plot size may vary (depending on the plotter). It is possible to output several plots automatically to each page, or several plots may be formatted on a page by outputting each separately with different plotting areas defined on the plotter page (see below.) Plot size and proportions may also be changed by altering the axis lengths from the default values of 25 x 20 cm (item 16 in the 'define main plot parameters' option of the GDA program - see above). This must be done before generating the metafiles, but note that it does not apply to triangular plots or legends.

The menu, which appears after typing PLOT, is:

(1) Select plot (metafile) (1-99).

(2) Select speed of connected plotter (1-50 cm/sec; default = 10; a slow speed improves the quality of straight lines, but does not affect the overall time taken to produce a plot very much, as the slowest pen speed is always used for curved lines).

(3) Select rotation of connected plotter (0 = normal; 1=90°; the latter rotates the whole plot by 90°, but also changes its proportions; the distortion may be eliminated by setting the plotting area (see 5) to 0.0 to 1.0 across by 0.0 to 0.5 up - in effect, this means that plots output to an A3 page plotter appear on an A4 size area).

(4) Define number of plots per page (1 to 5 across the page, 1 to 3 up the page; default is 1 plot per page; the plotter page is divided into equal areas, and one plot is output to each; for example, 2 x 2 (i.e., 4 plots per page) will produce 1 plot, of half the (linear) size, in each quarter of the page).

(5) Define plotting area within page (this can position each plot to a different part of the page; the following must be specified (including decimal point):

min. across page (0.0 to 1.0)
max. across page (0.0 to 1.0)
min. up page (0.0 to 1.0)
max. up page (0.0 to 1.0);

each plot will appear in the specified part of the page (e.g., 0.0 to 0.5 across and 0.0 to 0.5 up will be at bottom left, in the same position, in fact, as the bottom left hand plot when 4 per page is specified under item 4) at a reduced size (in this example, 50% of the original size); note that if the proportions of the specified part of the page are changed (e.g., 0.0 to 0.5 across and 0.0 to 0.3 up), then the proportions of the plot (including text and symbols) will be similarly changed; note also that the specified maximum must be greater than the minimum, although the latter does not have to be 0.0; the default values are 0.0 to 1.0 both across and up the page, i.e., the output plot occupies the whole page; the page size is set to 40.4 x 28.5 cm (about A3) for direct output to the an HP plotter (see INSTALLATION), whereas for output via HPGL files to an offline plotter or laser printer the page size is normally set to A4 (this can be changed)).

(6) Switch output of plots to HPGL on file (appears if output is connected to plotter),
or
Switch output to directly connected plotter (appears if output is to HPGL files).

(7) Output selected plot (i.e., plot specified in item 1 - either directly to plotter or to HPGL file).

(8) Output all plots starting at selected one (to plotter, when more than one is to be output per page, or to HPGL files).

(9) Delete all metafiles (plots).

(10) Delete all HPGL files.

There are thus two basic ways in which plots can be formatted on the plotter page, either by specifying a particular number of plots per page (item 4) or by defining different plotting areas on the page (item 5). It is also possible to use a combination of these. For instance, to output 2 plots to an A4 page (as opposed to 4 to an A3 page) on an A3 page plotter, select 2 (1 across by 2 up) plots per page, and set the plotting area to 0.0 to 0.5 across by 0.0 to 1.0 up the page. If the plotting area is not defined in this way the 2 plots will be stretched out in the X direction, as the plotter page is automatically divided equally into the specified number of sections.

Examples of other ways of formatting plots are given in Figure 7, which were prepared on a Graphtec plotter.

Figures 7A-C are stacked XY plots with different X-axis elements. For each XY plot in each stack, the number of plots per page is set to one, but the plotting area for each is specified so that the plot appears in the correct position on the page. For five stacked plots (Figure 7A), the axis lengths (X, Y) (item 16 on the plot parameters menu of the GDA program) are set to 40 x 12 cm. (Note that this causes the Y-axis label to move off the screen, but it will appear on the plot). The plotting area across the page is set to 0.1 to 0.4 in each case (this ensures that the Y-axis label appears on the plot), and the area up the page was set to 0.00 to 0.30, 0.175 to 0.475, 0.35 to 0.65, 0.525 to 0.825, and 0.70 to 1.00, respectively, for the five consecutive plots. Note that the proportion of the page specified both across and up in each use is the same (i.e., 0.3), so that the final plot is not distorted. Note also that the plotting area specified for each plot partly overlaps the next one in order to reduce the

gap between plots. Symbol and axis label sizes were enlarged somewhat from the default values, to 0.85 and 1.25cm, respectively.

Similar stacks of 3 or 4 plots may be produced by choosing suitable limits to the plotting area for each plot. The following table summarises the values used to produce the stacked plots shown in Figures 7A-C.

No of stacked plots	Axes (cm) X	Y	Plotting area within page across	up	Symbol Size (cm)	Label Size (cm)
5	40	12	0.10-0.40	0.00-0.30 0.175-0.475 0.35-0.65 0.525-0.825 0.70-1.00	0.85	1.25
4	36	15	0.10-0.43	0.00-0.33 0.22-0.55 0.44-0.77 0.66-0.99	0.75	1.20
3	30	17	0.10-0.50	0.00-0.40 0.30-0.70 0.60-1.00	0.63	1.10

These parameters can, of course, be varied to suit individual requirements. Thus, the spacing between plots can be increased (or reduced) by slightly reducing (or increasing) the length of the Y axis. Alternatively, the vertical spacing can be changed by slightly moving the plotting areas up or down. For example, the spacing of 2 standard plots output on a page, as in Figure 5, can be reduced by specifying slightly overlapping plotting areas (e.g., 0.0 to 0.5 and 0.43 to 0.93 up, by 0.0 to 0.5 across); however, note that each plot must be output separately (1 per page, not 4 per page). Larger plots can be produced by increasing the plotting area (across and up) in the same proportions, although this will obviously decrease the

number which can be fitted up the page. Figure 7D shows a triangular plot with the appropriate legend underneath output as a set of 2 plots per page. The legend may be positioned more centrally by outputting each plot separately and specifying the plotting area for the legend as 0.1 to 0.6 across by 0.05 to 0.55 up (Figure 7E). Of course, wider legends may not need to be moved across the page at all.

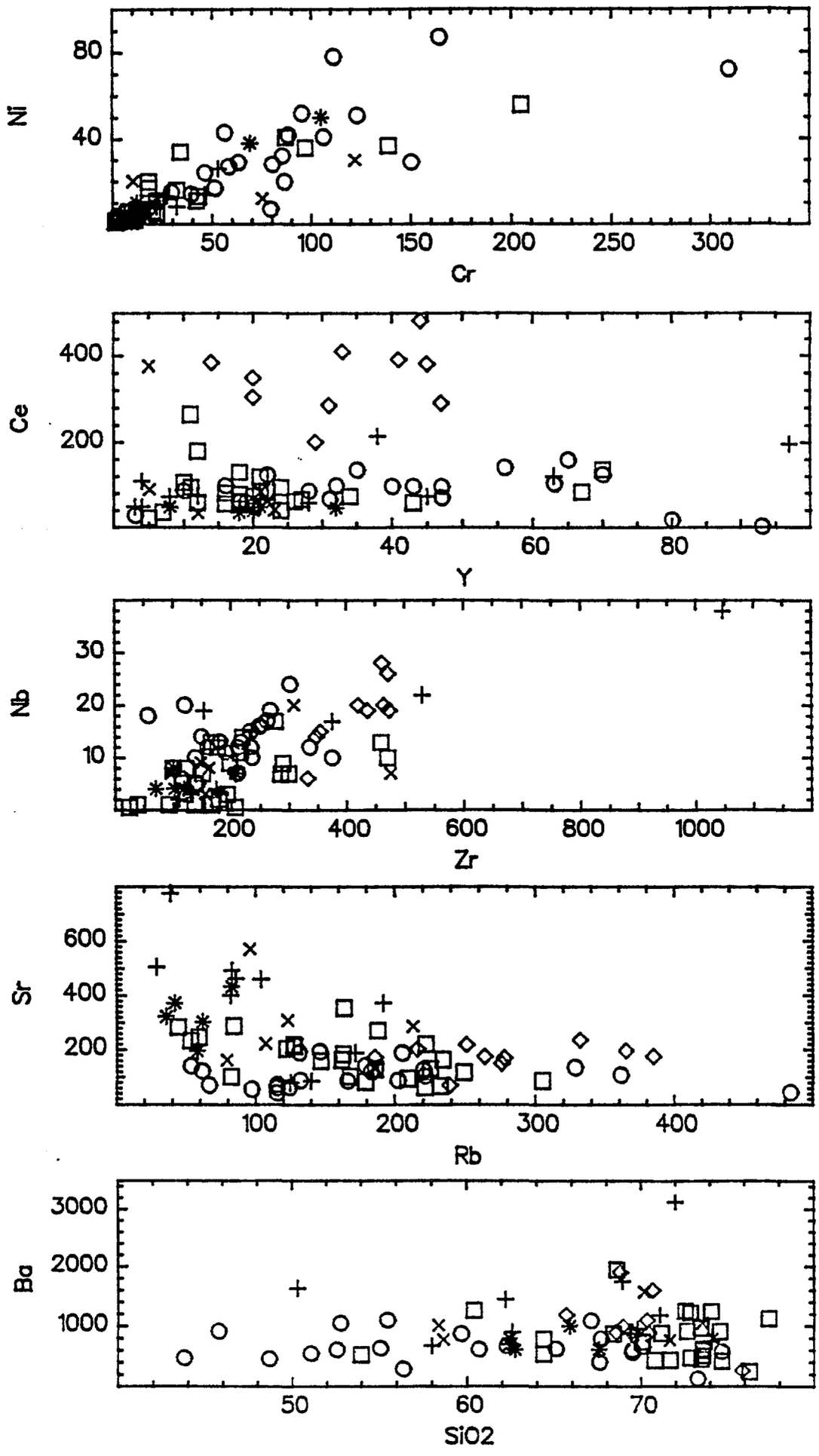

Ni
80
40
50
100
150
200
250
300
Cr
Ce
400
200
20
40
60
80
Y
Nb
30
20
10
200
400
600
800
1000
Zr
Sr
600
400
200
100
200
300
400
Rb
Ba
3000
2000
1000
50
60
70
SiO2

FIG. 7A

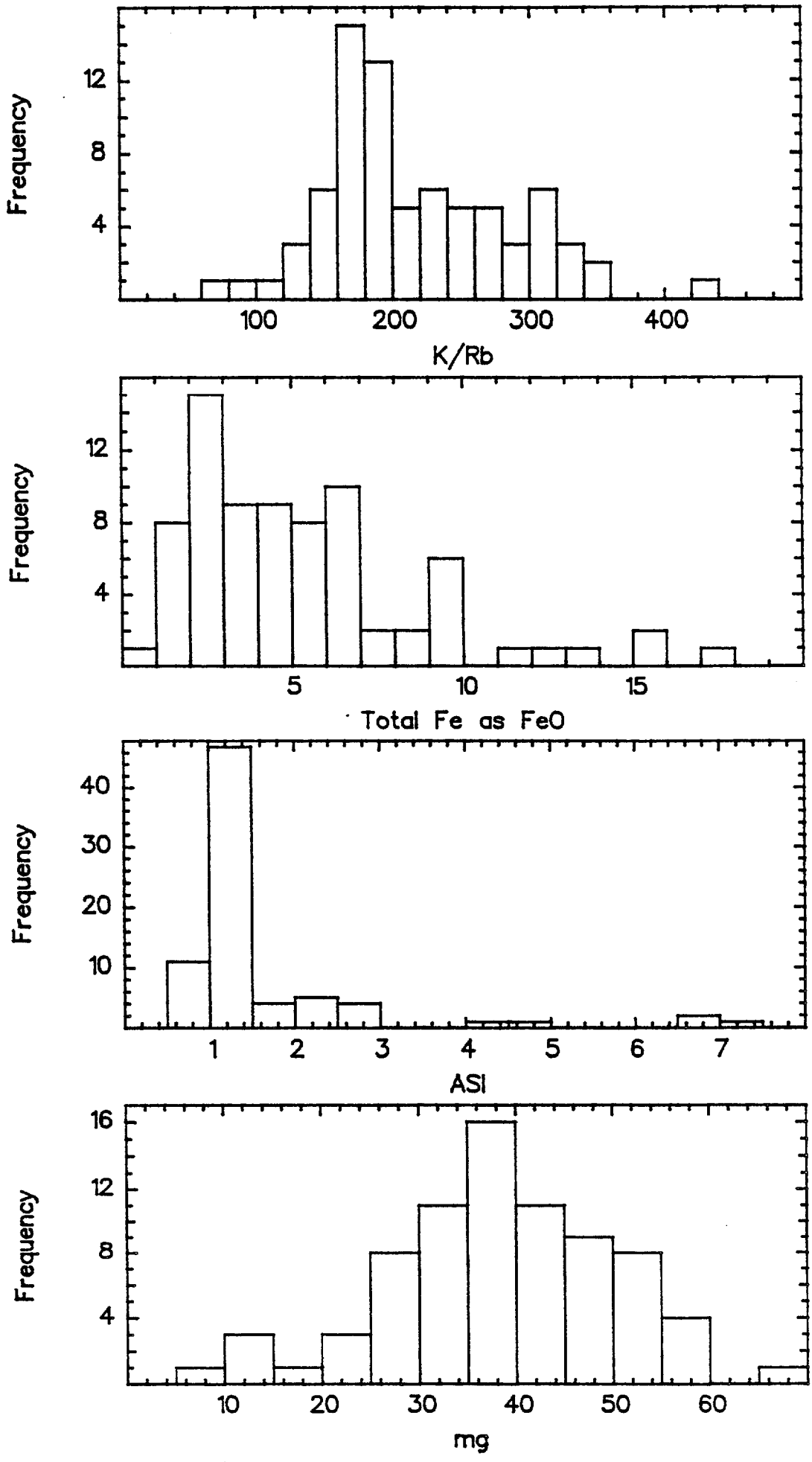

Frequency
12
8
4
100
200
300
400
K/Rb
Frequency
12
8
4
5
10
15
Total Fe as FeO
Frequency
40
30
20
10
1
2
3
4
5
6
7
ASI
Frequency
16
12
8
4
10
20
30
40
50
60
mg

FIG. 7B

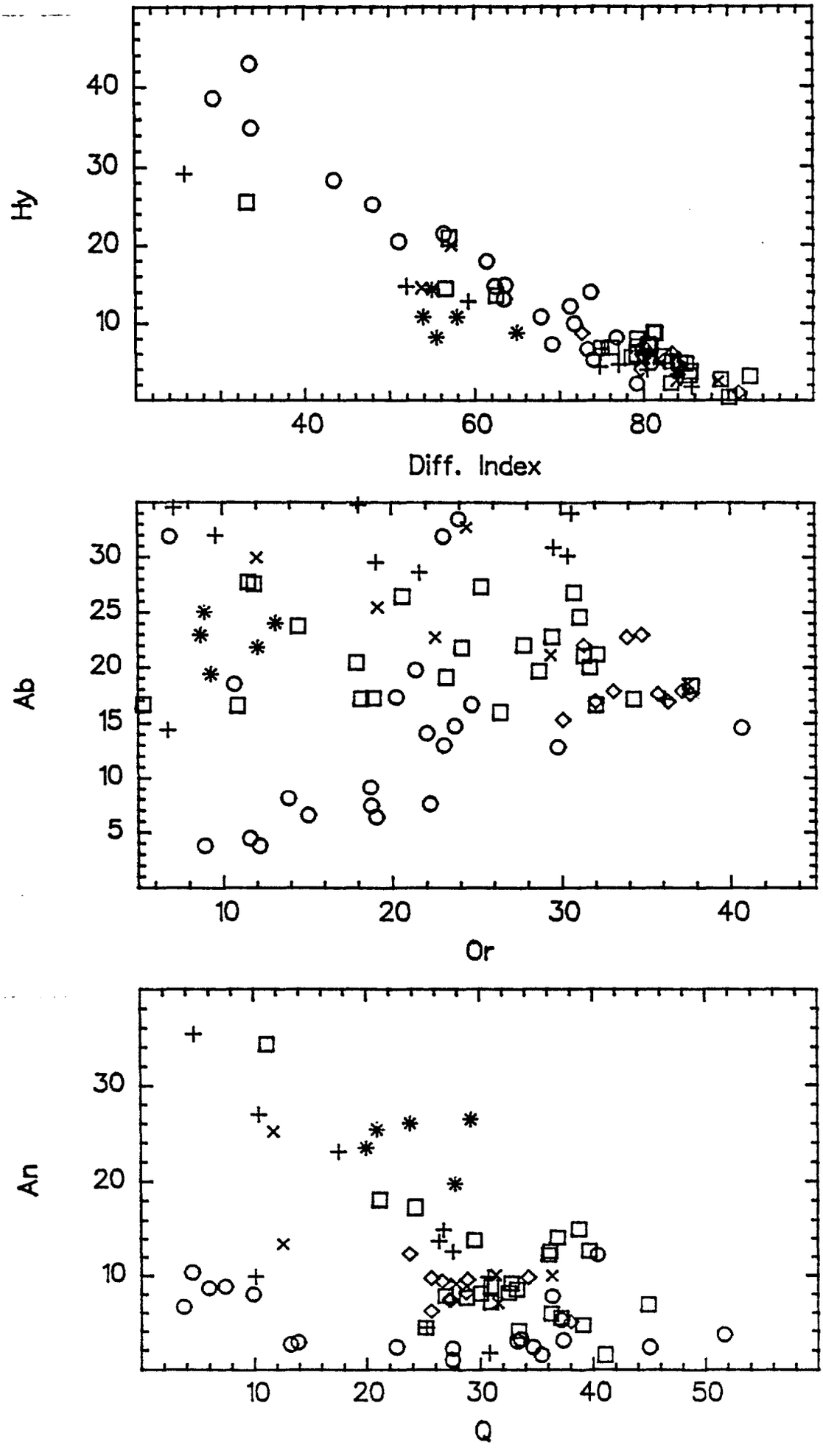

Hy
40
30
20
10
40
60
80
Diff. Index
Ab
30
25
20
15
10
5
10
20
30
40
Or
An
30
20
10
10
20
30
40
50
Q

FIG. 7C

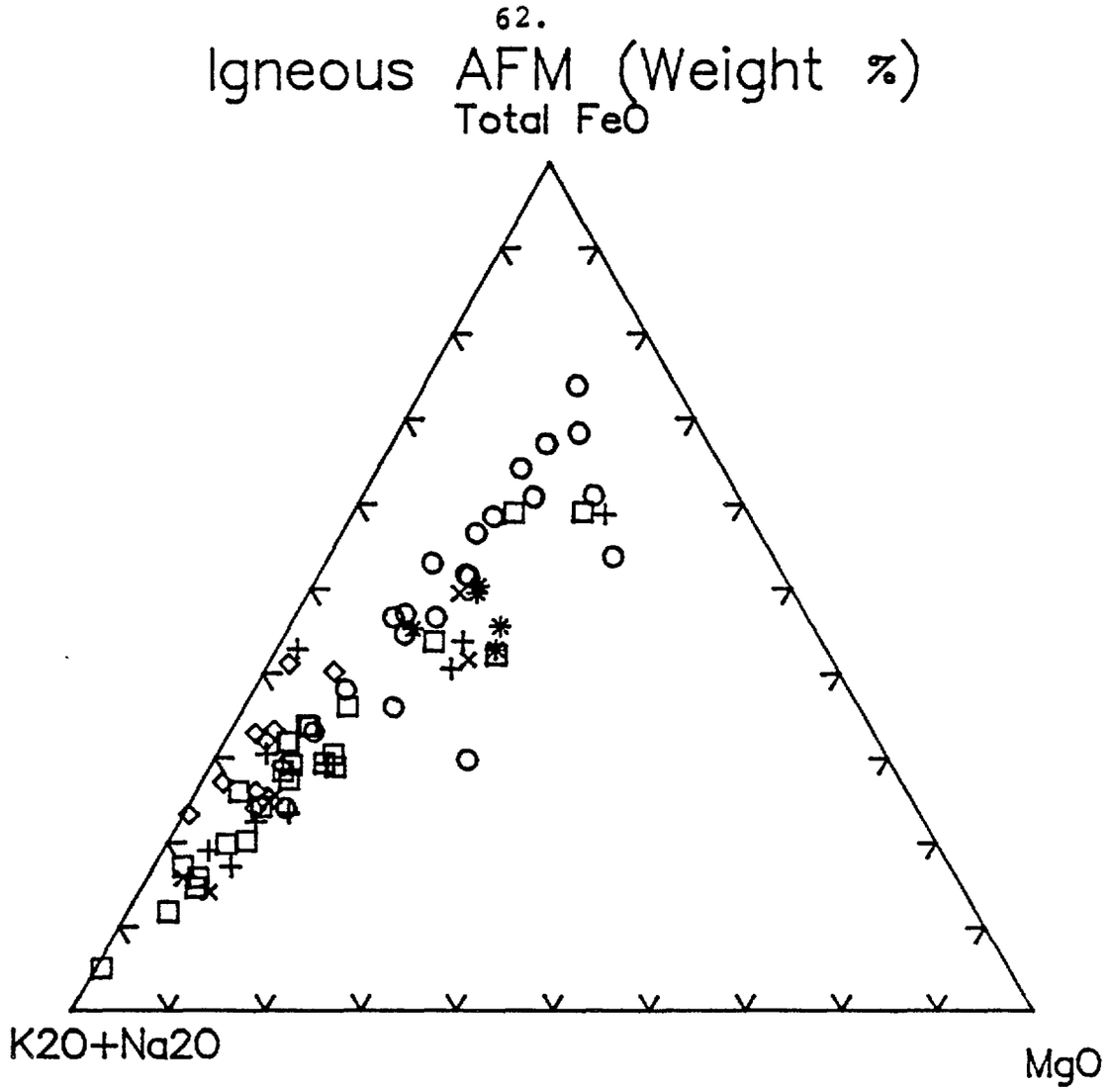

Igneous AFM (Weight %)
Total FeO
K20+Na20
MgO
Rauer Opx
Rauer Gt
Prydz Opx
Prydz Gt
Granite
Pelite

FIG. 7D

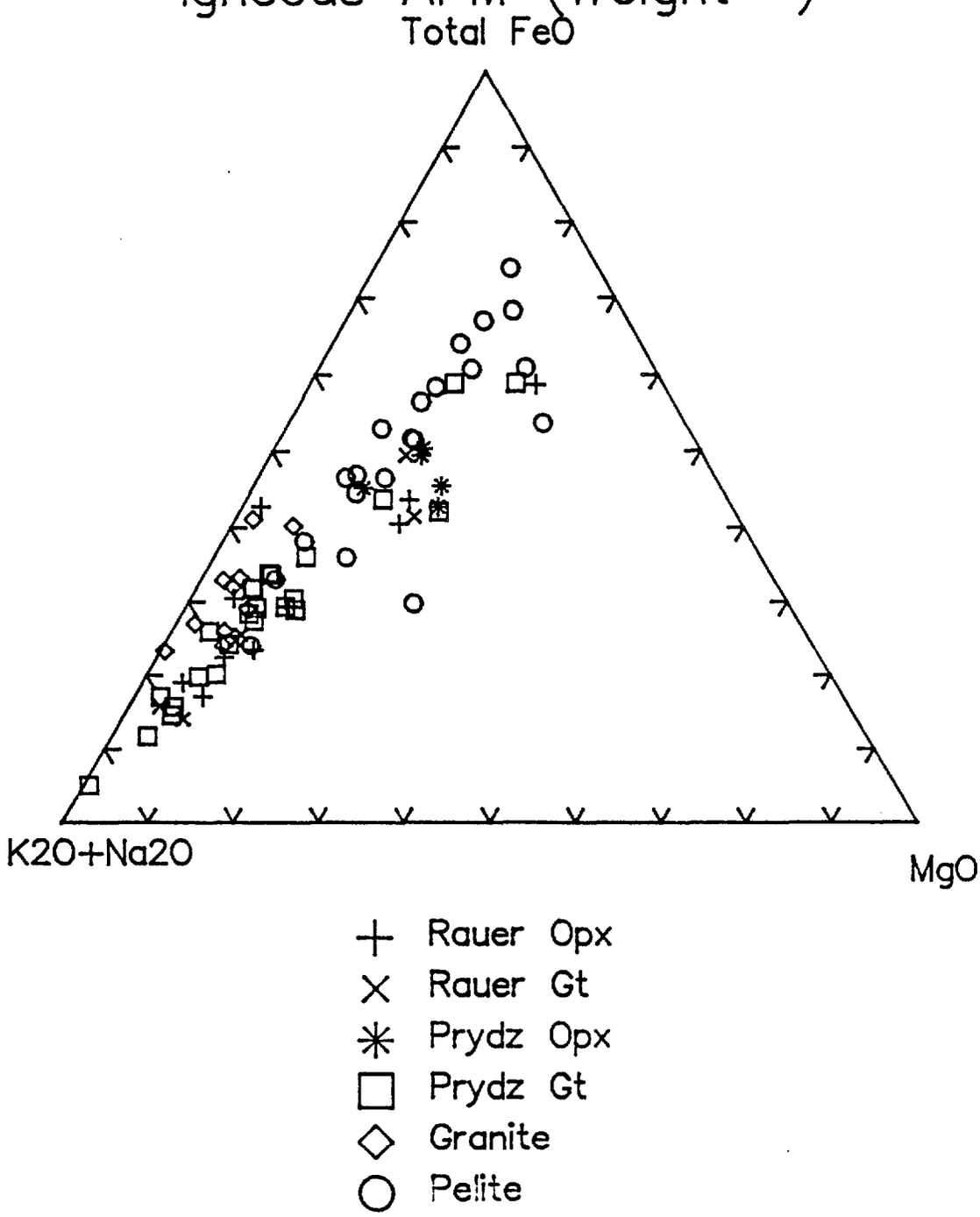

Igneous AFM (Weight %)
Total FeO
K2O+Na2O
MgO
Rauer Opx
Rauer Gt
Prydz Opx
Prydz Gt
Granite
Pelite

FIG. 7E

Figure 8 shows examples of good quality A4-size plots produced on a laser printer from HPGL files.

Figure 8A is a standard plot (i.e., with default axes, symbol and label sizes, etc.) output at 1 per page.

Figure 8B is a similar plot, except that smaller axes (17.5 x 14 cm) were used to produce a smaller plot, and the symbol, tick, and label sizes were reduced by 1/3 (to 0.34, 0.67, and 0.67cm, respectively). A graphics overlay file (KSIL.GRF - K_2O-SiO_2 classification of volcanic rocks) was added. Note that the same size plot could have been produced by retaining the default axes (25x20 cm) and symbol, etc. sizes, but setting the plotting area to 0.1 to 0.8 across by 0.1 to 0.8 up. A plot of this size could be photo-reduced by 30 or 40 percent to produce a publication-standard plot.

Figure 8C is an example of 4 plots output to one page. In this case, it was necessary to set the plotting area to 0.1 to 1.0 across by 0.1 to 1.0 up. This is because laser printer plots tend to be truncated at the bottom (particularly the X-axis labels). It is advisable to check the laser printer being used to see if this is a problem.

Figure 8D is an example of a stacked plot, analagous to Figure 7C. All parameters were set as for Figure 7C (see above Table), except that the plotting areas were defined as follows: 0.2 - 0.56 across by

0.10 - 0.46
0.37 - 0.73
0.64 - 1.00 up.

Note that each 'up' co-ordinate was obtained by multiplying those given in the above Table by 0.9 and adding 0.1. This ensures that the bottom X-axis label is not truncated. The range across the page was reduced by the same factor (0.9).

Figure 8E is a stack of 5 plots. Axis lengths were set to X=15.0 cm and Y = 28.0 cm, axis labels and ticks to 0.5cm, and symbols to 0.3 cm. The plotting area was set to 0.1 to 1.0 each way. The negative of the mg value

was used for the X-axis dataset. Setting Y = 28.0 cm is about the maximum which will fit on the page.

Figure 8F is an example of a plot with added title and different font.

In general, to output more than one plot per page to the laser printer (as in Figures 8C and D) it is necessary to copy all the required plots in one command, e.g.,

```
copy A:*.HPG com1 or print A:*.HPG
```

This avoids having to feed in the same A4 page for each plot. However, note that only the plot files required for a single page must be on the floppy disk as all such files with names in this format (*.HPG) will be output. If only some of the plot files on a floppy are required, they may be specified individually (before plotting of the first is complete) and queued.

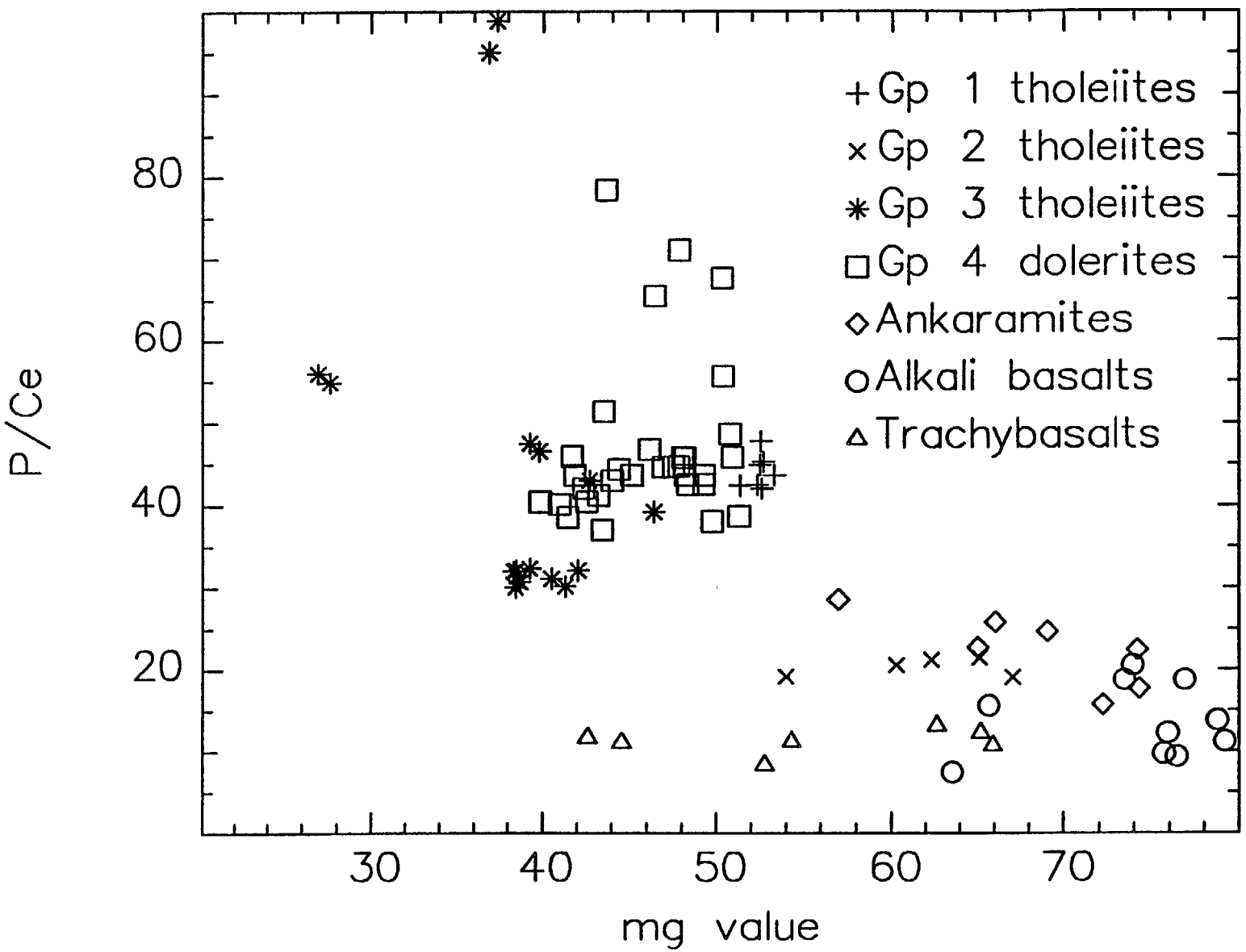

+Gp 1 tholeiites
×Gp 2 tholeiites
*Gp 3 tholeiites
□Gp 4 dolerites
◇Ankaramites
○Alkali basalts
△Trachybasalts
P/Ce
80
60
40
20
30
40
50
60
70
mg value

FIG. 8A

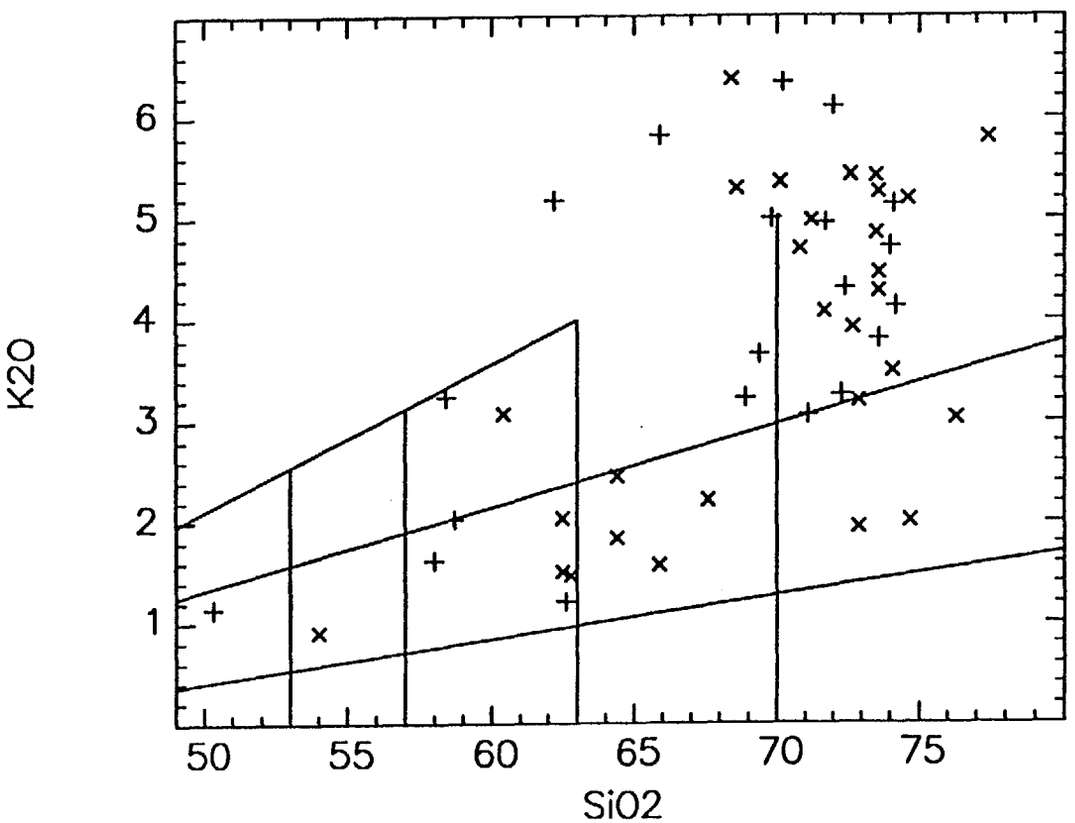
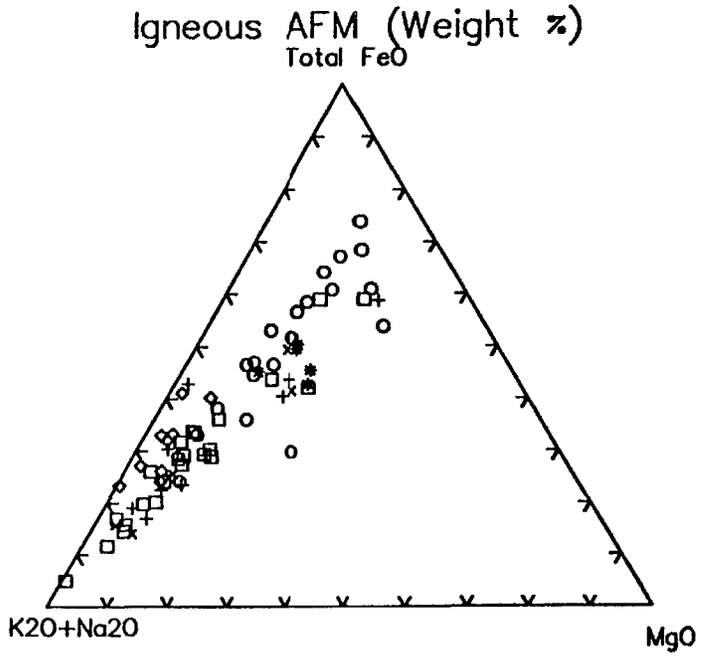
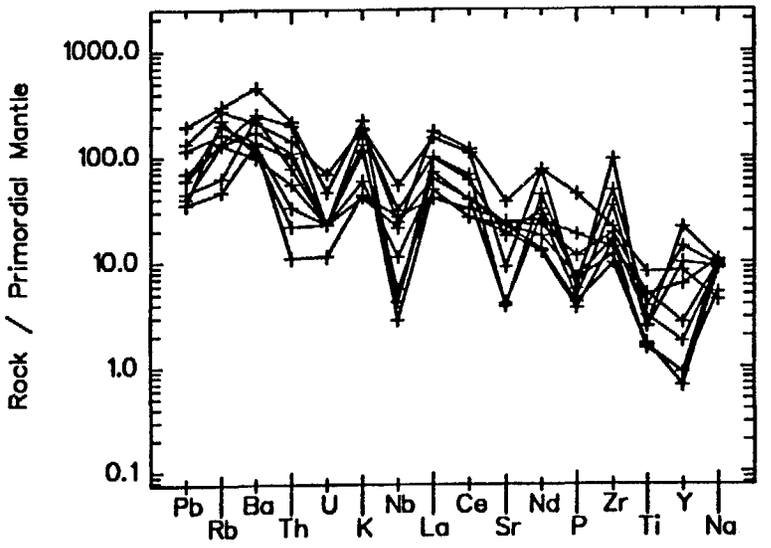
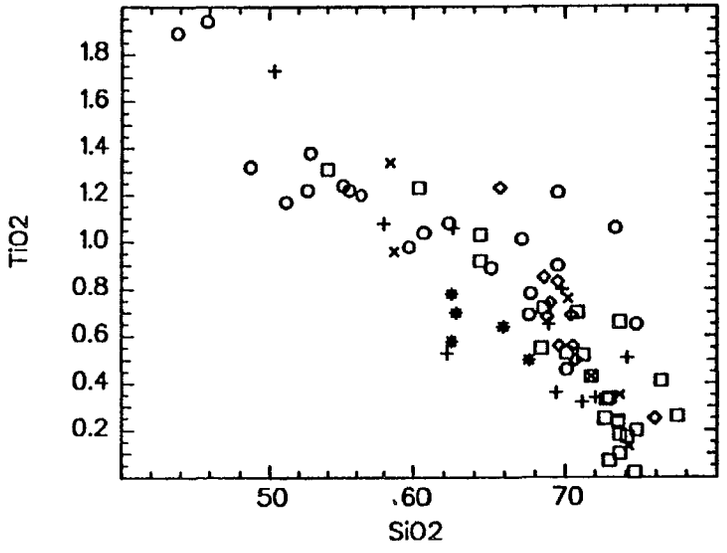


FIG. 8B


Igneous AFM (Weight %)
Total FeO
K2O+Na2O
MgO


Rock / Primordial Mantle
1000.0
100.0
10.0
1.0
0.1
Pb
Rb
Ba
Th
U
K
Nb
La
Ce
Sr
Nd
P
Zr
Ti
Y
Na


TiO2
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
50
60
70
SiO2

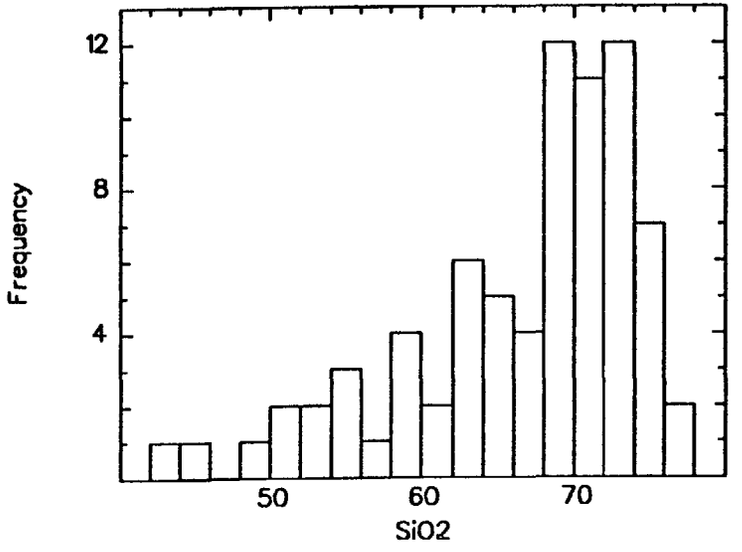

Frequency
12
8
4
50
60
70
SiO2

FIG. 8C

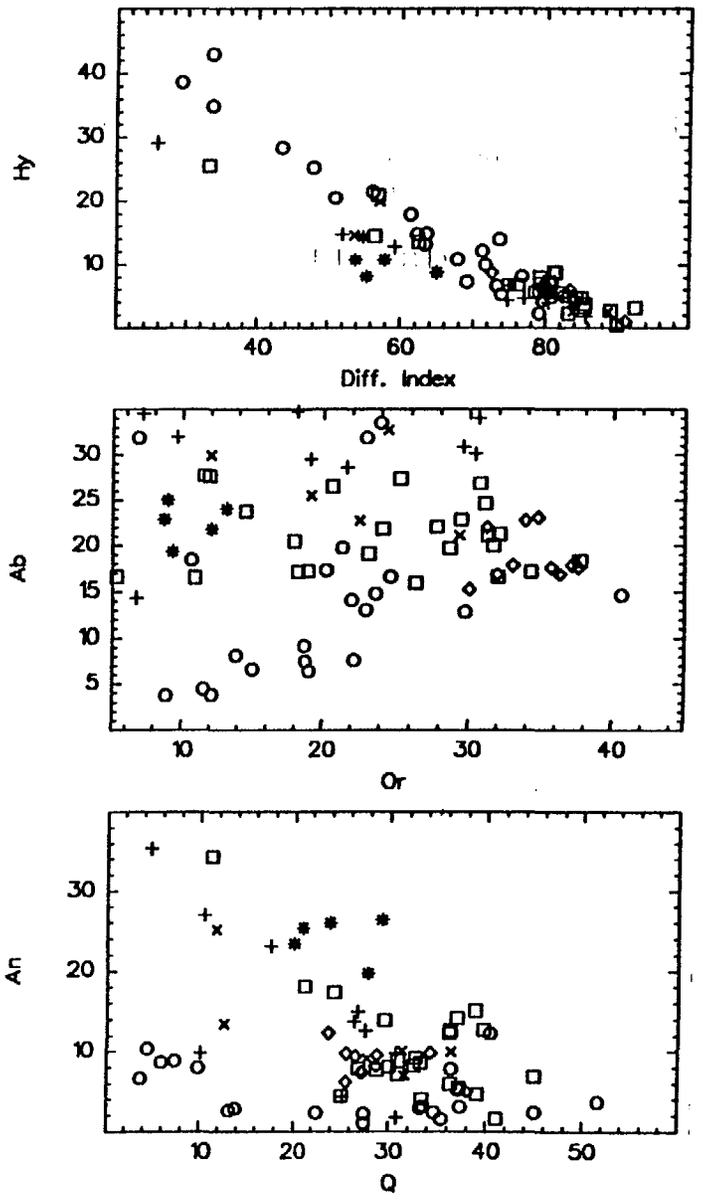

Hy
40
30
20
10
40
60
80
Diff. Index
Ab
30
25
20
15
10
5
10
20
30
40
Or
An
30
20
10
10
20
30
40
50
Q

FIG. 8D

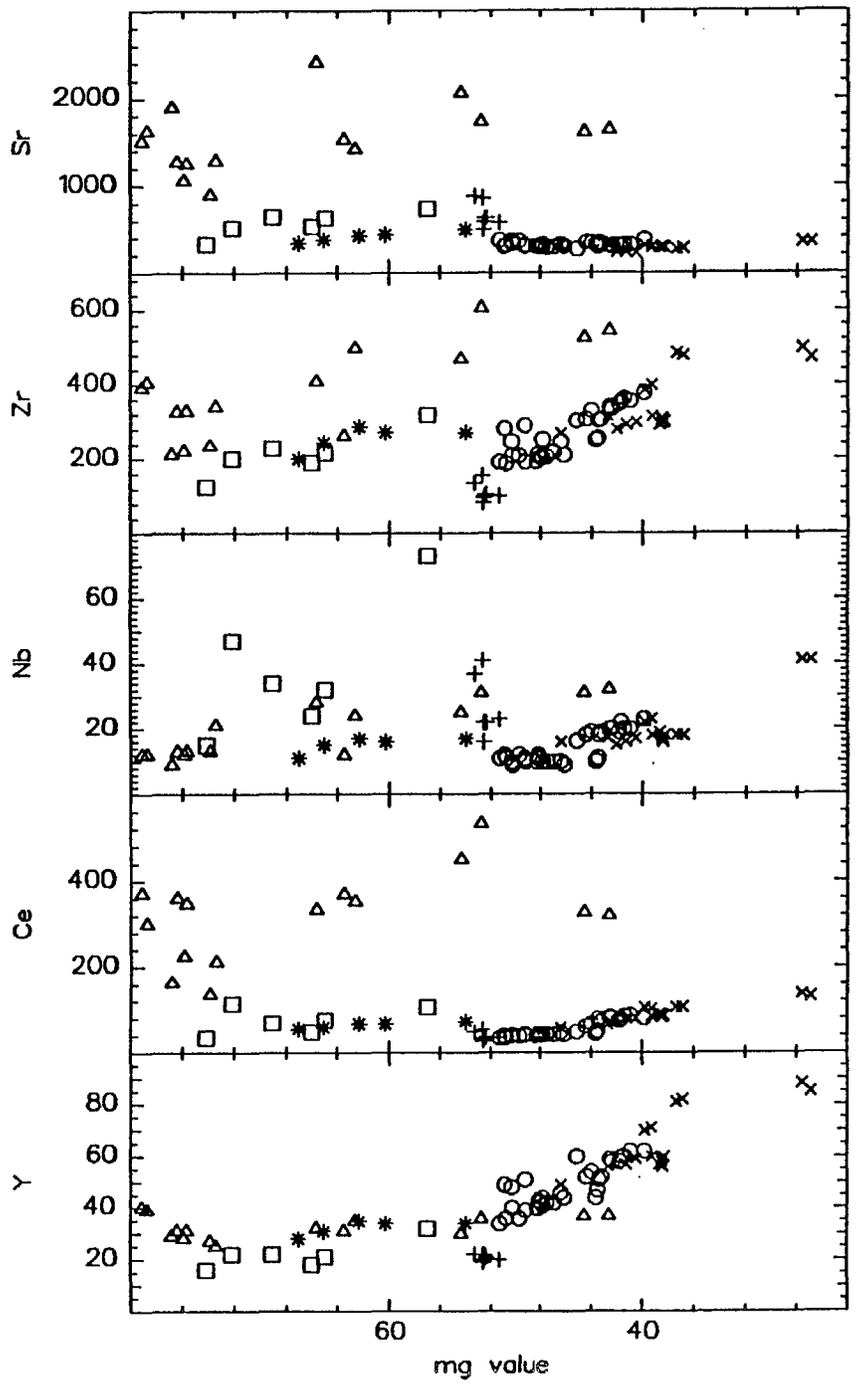

Sr
2000
1000
Zr
600
400
200
Nb
60
40
20
Ce
400
200
Y
80
60
40
20
60
40
mg value

FIG. 9C

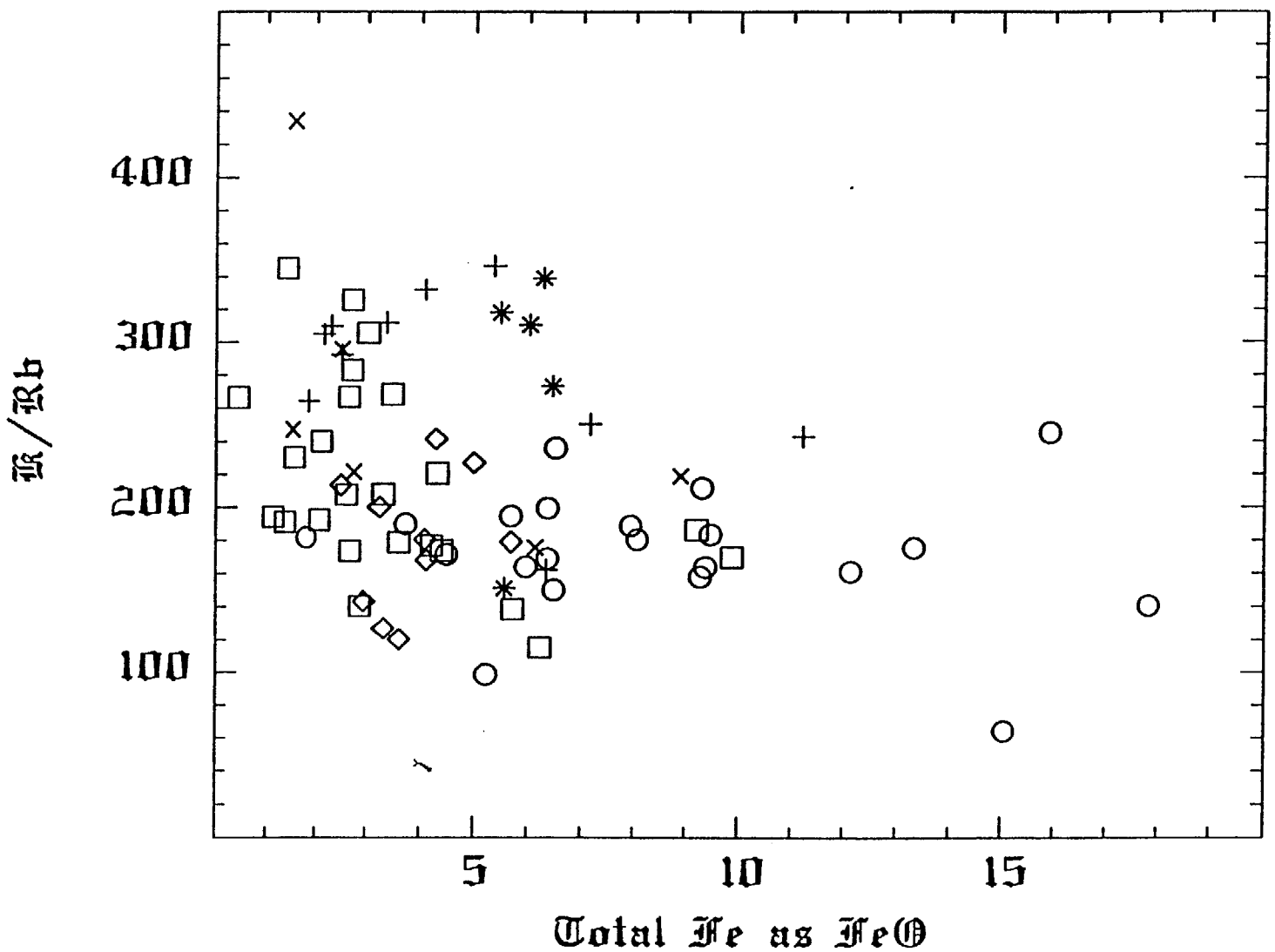

Ye Olde Englishe Plotte
400
300
200
100
K/Rb
5
10
15
Total Fe as FeO

FIG. 8F

7. TABLE

This program enables tables of geochemical data, including major and trace elements, CIPW norms, and element ratios or other expressions to be printed.

Elements can be dropped from any of the parts, and there are options for defining arithmetic expressions and for control of headings and layout. Printout of CIPW norms must be specified, if required. Samples are displayed by groups, except for the single sample option.

The standard report file REPORT.RPT gives corrections to field names for printing (e.g., upper to upper and lower case), defines which fields are in each part (major, trace, or description), as well as their orders, and gives other information such as factors for converting ppm to weight percent oxide. The latter are used to calculate 'rest' to add to the total of major oxides. The program also calculates corrections to this total for F, Cl, and S contents.

The standard report file REPORT.RPT is as follows:

```
Report definition file REPORT.RPT
major elements
15
SIO2        Si02
TIO2        Ti02
AL2O3       Al203
FE2O3       Fe203
FEO         Fe0
MNO         Mn0
MGO         Mg0
CAO         Ca0
NAO2        Na20
K2O         K20
P2O5        P205
H2O+        H20+
H2O-        H20-
CO2         C02
LOI         LOI
Trace elements

47
BA          Ba      1.1165
LI          Li      2.15253
RB          Rb      1.0936
SR          Sr      1.1826
```

PB	Pb	1.07722
TH	Th	1.1379
U	U	1.13443
ZR	Zr	1.35079
NB	Nb	1.43053
Y	Y	1.26994
LA	La	1.17277
CE	Ce	1.17128
ND	Nd	1.16638
PR	Pr	1.20817
SC	Sc	1.53384
V	V	1.78518
CR	Cr	1.46156
MN	Mn	0.00000
CO	Co	1.27148
NI	Ni	1.27256
CU	Cu	1.25178
ZN	Zn	1.24471
SN	Sn	1.2696
W	W	1.26108
MO	Mo	1.33353
GA	Ga	1.34422
AS	As	1.3203
S	S	1.0
C	C	1.0
F	F	1.0
CL	CL	1.0
BE	Be	2.77531
B	B	3.2201
AG	Ag	1.0742
AU	Au	1.0
HG	Hg	1.0798
BI	Bi	1.1148
SB	Sb	1.19713
HF	Hf	1.17928
TA	Ta	1.22106
CS	Cs	1.06023
GE	Ge	1.4408
BR	Br	1.0
SE	Se	1.0
PT	Pt	1.0
PD	Pd	1.0
IR	Ir	1.0

Description fields

16

SAMPNO	Sample number
STATE	State
REGION	Region
LOCALITY	Locality
STRATGROUP	Stratigraphic group
STRATUNIT	Stratigraphic unit
MAPSYMBOL	Map symbol
LITHOLOGY	Lithology
MAPNAME	Map name
GRIDREF	Grid reference
DRILLHOLE	Drill hole

DEPTH	Depth
AGE	Age
BIBLIOREF	Bibliographic ref.
ORIGINATOR	Originator
OTHERDATA	Other data

This file may be edited to include further elements, if required, but must include both major and trace elements and description fields.

Note that the various options (4-19) must be specified before displaying or generating the report.

The menu, obtained by typing TABLE, is as follows:

(1) Generate report on print file TABLE.PRN

(2) Display report on screen.

(3) Display for single samples on screen (headings, major and trace elements only; sample number must be specified).

(4) Select major elements (all are included by default).

(5) Select trace elements (only those for which data is present are queried; all these are included by default).

(6) Select CIPW norm minerals (including normative expressions).

(7) Specify descriptive fields.

(8) Specify CIPW norm parameters (see under GDA).

(9) Select groups to be printed or displayed (printing of each group starts on a new page).

(10) Specify range of assigned samples (only assigned samples are printed, in the order in which they appear in the GDA file; only the groups selected in (9) are included).

(11) Specify group titles (group names used in GDA may be expanded, if

required).

(12) Specify if trace element title line is required ('trace elements in parts per million').

(13) Specify number of samples per printer page (1-10; up to 5 for A4 page, 10 for wide printer; default is 5).

(14) Specify number of lines on printer page (10-500; default of 60 gives a space at top and bottom of each page; each group of data (headings, major elements, CIPW norms, trace elements) will start on a new page if it cannot all be fitted on the previous page).

(15) Print values for standard expressions (as for GDA).

(16) Print values for typed-in expressions (a dataset number and label must be specified for each).

(17) Print standard datasets (as for GDA).

(18) Include page header (i.e., title on each page).

(19) Print page count (i.e., number pages; default is 'off').

(20) Change GDA file.

The file TABLE.PRN may be edited with a word-processor, if required, before printing. Two examples of such tables are given below.

Rauer Islands Opx Gneisses

Sample number	81285103	81285115	81285119	81285120	81285124
State	Antarctica	Antarctica	Antarctica	Antarctica	Antarctica
Region	Prydz Bay Coast	Prydz Bay Coast	Prydz Bay Coast	Prydz Bay Coast	Prydz Bay Coast
Locality	Filla Island	SE Rauer Group	Torckler Island	E Rauer Group	Hop Island
Lithology	Bi-Op-QzPl gneiss	Ol-Op-Cp granite gn	Op-Kf-QzPl gneiss	Op-Cp-QzPl gneiss	Cp-Qz-OpPl gneiss
Age	Protero	Protero	Protero	Protero	Proterc
Bibliographic ref.	15,18	15,18	15,18	15,18	15,18
Originator	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton
Other data	Rauer Op	Rauer Op	Rauer Op	Rauer Op	Rauer Op
SiO2	62.60	62.20	68.90	74.10	50.30
TiO2	1.06	.53	.65	.51	1.73
Al2O3	16.50	15.84	14.26	12.05	17.00
Fe2O3	.78	2.59	.61	1.06	.18
FeO	4.66	4.83	2.81	1.21	11.06
MnO	.12	.17	.05	.05	.18
MgO	2.57	.36	1.38	.54	5.04
CaO	5.18	3.34	3.19	1.49	8.90
Na2O	4.08	4.02	3.49	3.56	1.70
K2O	1.21	5.18	3.23	5.14	1.14
P2O5	.40	.12	.16	.10	.96
H2O+	.54	.44	.44	.48	.31
Rest	.26	.44	.34	.20	.45
Total	99.96	100.06	99.51	100.49	98.95

C.I.P.W. norms

Q	17.53	10.10	26.36	30.82	4.68
C	.02	-	-	-	-
Or	7.15	30.61	19.09	30.37	6.74
Ab	34.52	34.02	29.53	30.12	14.38
An	23.08	9.88	13.70	1.72	35.39
Di	-	5.16	.89	4.02	2.09
Di(CaMg)	-	.74	.46	2.90	.94
Hd	-	4.42	.43	1.12	1.15
Hy	12.78	4.37	6.67	-	29.14
En	6.40	.55	3.22	-	12.12
Fs	6.38	3.82	3.44	-	17.02
Mt	1.13	3.75	.88	1.54	.26
Il	2.01	1.01	1.23	.97	3.29
Ap	.95	.28	.38	.24	2.27
Diff. Index	59.20	74.73	74.98	91.32	25.80
Colour Index	15.93	14.29	9.68	6.54	34.78
Pl	57.61	43.89	43.24	31.84	49.77
Norm Plag Comp	40.07	22.50	31.70	5.40	71.10
mg number	49.57	11.72	46.67	44.30	44.81

Trace elements in parts per million

Ba	905	1448	1750	746	1635
Li	22	12	12	4	9
Rb	29	172	86	140	39
Sr	506	189	462	86	776
Pb	7	27	12	7	9
Th	1	13	18	2	7
U	<.50	1.50	.50	.50	.50
Zr	153	1047	181	375	236
Nb	19	38	3	17	15
Y	28	97	8	45	38
La	28	106	50	43	122
Ce	58	197	71	72	215
Nd	34	101	24	38	101
Sc	17	4	6	3	35
V	90	3	54	12	255
Cr	53	4	27	6	32
Ni	26	2	13	6	8
Cu	19	10	34	11	19
Zn	97	154	40	23	131
Ga	22	29	14	13	21
As	<.50	1.00	.50	.50	<.50
F	-	<200	-	-	-
Be	2	4	1	2	3
ASI	1.00	.88	.97	.87	.95
Total Fe as FeO	5.36	7.16	3.36	2.16	11.22
K/Rb	346.35	250.00	311.77	304.77	242.64
Ce/Y	2.07	2.03	8.88	1.60	5.66
Zr/Nb	8.05	27.55	60.33	22.06	15.73

Alkali basalts

Sample number	86285611	86285637	86286055	86285957	86285922	86285921	86285917	86285918	86285912	86285677
State	Antarctica	Antarctica	Antarctica	Antarctica	Antarctica	Antarctica	Antarctica	Antarctica	Antarctica	Antarctica
Region	Bunger Hills	Bunger Hills	Bunger Hills	Bunger Hills	Bunger Hills	Bunger Hills	Bunger Hills	Bunger Hills	Bunger Hills	Bunger Hills
Locality	Geografov Island N	Thomas Island SW	Pluton Island E	W Lake Dolgoe	C Taylor Islands	C Taylor Islands	C Taylor Islands	C Taylor Islands	1km SE of Edgeworth David	W Lake Dolgoe
Lithology	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt	Alkali olivine basalt
Originator	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton	J. Sheraton
SiO2	46.20	47.30	47.30	45.00	46.20	46.00	48.70	48.30	45.90	46.10
TiO2	.91	1.16	1.01	.92	1.05	1.05	1.01	1.10	1.47	.93
Al2O3	11.75	16.95	12.23	12.23	11.16	11.06	13.22	14.29	13.98	12.96
Fe2O3	2.84	3.65	2.72	3.21	2.28	2.23	1.57	1.84	3.36	3.43
FeO	5.96	4.69	4.90	4.27	6.44	6.31	6.33	5.59	4.98	3.98
MnO	.14	.13	.12	.13	.14	.13	.13	.12	.14	.14
MgO	13.49	6.63	11.05	12.98	13.13	12.36	10.47	9.56	7.30	12.49
CaO	7.62	8.16	9.79	6.82	8.02	8.60	8.79	7.28	8.49	6.91
Na2O	1.58	2.94	1.61	1.75	1.54	1.53	2.03	2.12	2.58	1.91
K2O	4.30	2.34	3.78	4.78	3.80	3.76	3.36	4.92	5.14	4.89
P2O5	.70	.63	.63	.95	.77	.77	.64	.91	1.19	.95
H2O+	1.94	1.19	1.68	1.84	1.79	2.04	1.67	1.45	1.04	1.88
H2O-	.08	.14	.14	.03	.07	.23	.07	.05	.11	.10
CO2	.34	3.18	1.68	2.74	2.45	2.72	.79	.67	2.61	1.68
Rest	1.52	1.05	1.13	1.76	1.30	1.30	1.05	1.08	1.77	1.58
Total	99.37	100.14	99.77	99.41	100.14	100.09	99.83	99.28	100.06	99.93
O=F,S,Cl	.19	.08	.13	.09	.10	.10	.08	.06	.14	.10
Total	99.18	100.06	99.64	99.32	100.04	99.99	99.75	99.22	99.91	99.83

C.I.P.W. norms

Or	25.46	13.85	22.39	28.33	22.51	22.27	19.90	29.15	30.44	28.98
Ab	3.91	23.21	7.24	2.33	7.87	7.22	15.68	9.90	2.14	3.57
An	12.69	26.76	15.29	12.44	12.75	12.63	17.78	15.33	12.49	13.31
Ne	4.81	.50	3.24	5.87	2.45	2.76	.16	4.08	9.68	5.99
Di	18.05	9.14	24.17	14.13	18.97	21.36	18.50	13.20	19.89	13.56
Di(CaMg)	14.32	6.11	18.98	11.46	14.91	16.68	14.10	10.08	13.99	10.95
Hd	3.73	3.03	5.19	2.67	4.06	4.68	4.40	3.13	5.89	2.61
Ol	25.22	15.65	17.74	24.62	24.37	21.97	19.16	18.73	12.69	23.83
Fo	18.96	9.61	13.18	19.01	18.13	16.21	13.74	13.45	8.27	18.31
Fa	6.26	6.04	4.56	5.61	6.25	5.76	5.43	5.28	4.42	5.52
Mt	2.09	1.96	1.81	1.77	2.09	2.05	1.90	1.78	1.97	1.74
Il	1.73	2.20	1.92	1.75	1.99	1.99	1.92	2.09	2.79	1.77
Ap	1.71	1.53	1.52	2.35	1.87	1.87	1.55	2.21	2.93	2.34
Pr	.65	.23	.22	.15	.30	.31	.15	.17	.33	.20
Diff. Index	29.37	37.07	29.62	30.66	30.38	29.50	35.58	39.04	32.59	32.55
Colour Index	47.96	29.18	46.08	42.67	47.93	47.92	41.80	36.11	37.75	41.28
Norm Plag Comp	76.43	53.55	67.87	84.19	61.83	63.61	53.14	60.77	85.36	78.83
mg number	76.86	63.54	75.92	79.17	76.42	75.70	73.92	73.45	65.66	78.75

Trace elements in parts per million

Ba	4840	3950	4510	7280	4470	4360	3860	4240	6820	6060
Rb	129	69	128	213	139	142	114	189	180	213
Sr	1892	1526	1057	1507	1268	1245	893	1280	2410	1621
Pb	36	89	36	102	64	66	46	25	100	110
Th	13	50	36	76	42	42	23	58	42	76
U	2.50	5.00	5.00	9.00	6.00	5.00	4.50	7.50	6.00	10.00
Zr	212	262	221	392	327	328	234	340	408	406
Nb	9	12	12	12	13	13	13	21	28	12
Y	29	31	28	40	31	31	27	25	32	39
La	94	226	133	203	215	210	75	118	194	166
Ce	163	370	225	371	360	347	136	212	334	301
Nd	78	146	100	176	151	146	63	102	142	140
Sc	19	22	23	24	23	25	22	20	21	18
V	153	155	166	170	176	183	154	127	167	126
Cr	1082	20	1043	1231	953	1104	760	637	360	890
Ni	239	58	112	394	376	330	188	194	84	363
Cu	56	15	29	49	60	60	36	46	48	42
Zn	84	81	65	70	84	77	74	71	94	76
Ga	12	15	11	11	12	11	14	14	13	11
As	<.50	1.50	1.50	1.50	1.00	.50	<.50	<.50	3.50	2.00
S	3460	1230	1190	795	1600	1640	820	890	1790	1050
Cl	775	1010	540	2210	860	855	1620	685	2460	2070
P/Ce	18.75	7.43	12.22	11.18	9.34	9.69	20.54	18.74	15.55	13.78
K/Rb	276.67	281.48	245.11	186.26	226.91	219.77	244.63	216.06	237.01	190.55
Ti/Zr	25.73	26.54	27.40	14.07	19.25	19.19	25.68	19.40	21.60	13.73
Ce/Y	5.62	11.94	8.04	9.27	11.61	11.19	5.04	8.48	10.44	7.72

8. STATS

Statistical functions (mean, standard deviation, maximum, minimum, and optional correlation matrix), may be printed from file STATS.PRN, after specifying which options (2-9) are required. The same report definition file (REPORT.RPT) as in TABLE is normally used. The program is also used to generate a cluster analysis file for use in the CLUSTER program, details of which are given in the next section. Options 2-4, and 7-9 also apply in this case. The program is run by typing STATS and the menu is as follows:

(1) Generate statistics report (on file STATS.PRN).

(2) Select major elements (all by default).

(3) Select trace elements (all by default).

(4) Select groups (calculations are based on all selected groups).

(5) Specify group titles.

(6) Specify number of columns per page (1-10, depending on page size).

(7) Print values for standard expressions (as for GDA).

(8) Print values for typed-in expressions (dataset number and label must be specified).

(9) Drop samples (anomalous samples may be dropped from the calculations by specifying the appropriate sample number).

(10) Generate cluster analysis file (for use in CLUSTER program; a file name, ????.CLU, must be specified).

(11) Change GDA file.

A typical printout is given below.

GROUPS PROCESSED

Group 3 tholeiites
Group 4 dolerites

MEANS AND STANDARD DEVIATIONS

Element	Mean	Standard Deviation	Minimum	Maximum	Number of Items
SiO2	45.85	1.42	43.90	49.10	49
TiO2	3.51	.44	2.40	4.19	49
Al2O3	15.03	1.04	12.25	16.83	49
Fe2O3	3.76	.95	2.13	5.89	49
FeO	11.15	1.37	8.61	14.02	49
MnO	.23	.03	.18	.29	49
MgO	5.38	.97	2.78	6.92	49
CaO	8.35	.56	6.21	9.51	49
Na2O	3.04	.19	2.71	3.64	49
K2O	1.29	.45	.73	2.75	49
P2O5	.72	.44	.31	2.40	49
Ba	485.94	259.92	113.00	1524.00	49
Rb	29.33	13.21	6.00	53.00	49
Sr	302.29	32.09	224.00	373.00	49
Pb	8.78	3.24	3.00	15.00	49
Th	2.36	2.10	.50	8.00	49
U	.63	.34	.25	1.50	49
Zr	294.86	80.15	187.00	496.00	49
Nb	16.18	6.72	9.00	41.00	49
Y	53.90	12.71	34.00	88.00	49
La	27.67	13.00	12.00	63.00	49
Ce	67.29	26.14	35.00	136.00	49
Nd	42.06	16.29	23.00	83.00	49
Sc	26.78	3.81	18.00	36.00	49
V	252.78	63.13	29.00	349.00	49
Cr	54.76	28.38	1.00	120.00	49
Ni	54.02	24.36	1.00	105.00	49
Cu	38.22	8.17	21.00	65.00	49
Zn	133.96	18.87	99.00	179.00	49
Ga	21.47	1.49	19.00	24.00	49
As	.35	.23	.25	1.00	49
S	2128.78	624.71	500.00	4720.00	49
Cl	170.22	87.86	.00	430.00	46
Zr/Nb	19.15	3.51	11.49	26.83	49
Ce/Y	1.21	.23	.82	1.61	49

CORRELATION MATRIX

	SiO2	TiO2	Al2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O
SiO2	1.00									
TiO2	-.33	1.00								
Al2O3	-.07	-.47	1.00							
Fe2O3	.00	-.06	.11	1.00						
FeO	-.29	.49	-.65	-.68	1.00					
MnO	-.05	.34	-.89	-.14	.67	1.00				
MgO	-.66	-.18	.46	-.03	-.13	-.39	1.00			
CaO	-.54	.07	.45	-.02	-.22	-.38	.81	1.00		
Na2O	.10	-.38	.25	.02	-.05	-.02	-.30	-.47	1.00	
K2O	.57	.16	-.66	-.03	.30	.59	-.94	-.85	.23	1.00
P2O5	.06	.32	-.80	-.12	.55	.77	-.55	-.48	.04	.69
Ba	.59	-.01	-.59	-.06	.28	.55	-.89	-.86	.34	.94
Rb	.61	.33	-.51	-.04	.18	.34	-.91	-.68	.03	.88
Sr	-.33	-.48	.23	.01	-.00	.07	.19	.01	.46	-.07
Pb	.60	.33	-.56	-.04	.23	.43	-.91	-.71	.04	.90
Th	.69	.27	-.15	-.02	-.11	-.09	-.69	-.40	-.10	.56
U	.19	.08	-.13	-.19	.12	.10	-.16	-.05	-.11	.14
Zr	.15	.41	-.84	-.08	.57	.87	-.71	-.60	.11	.84
Nb	.37	.06	-.64	-.05	.41	.70	-.78	-.83	.37	.90
Y	.29	.39	-.83	-.08	.51	.83	-.79	-.64	.13	.88
La	.44	.31	-.68	-.02	.36	.62	-.91	-.77	.16	.96
Ce	.39	.37	-.73	-.05	.42	.68	-.89	-.75	.13	.95
Nd	.27	.39	-.81	-.11	.52	.79	-.81	-.67	.11	.91
Sc	-.42	.47	-.41	.06	.23	.32	.23	.37	-.49	-.12
V	-.51	.49	.01	.12	.04	-.07	.49	.55	-.56	-.47
Cr	-.37	-.27	.44	.02	-.24	-.34	.82	.72	-.18	-.83
Ni	-.31	-.34	.75	.02	-.41	-.75	.81	.62	-.11	-.89
Cu	-.35	-.04	.28	-.00	-.08	-.25	.71	.63	-.39	-.69
Zn	.30	.47	-.80	-.00	.48	.70	-.81	-.74	.07	.88
Ga	.02	.40	-.45	-.06	.38	.55	-.44	-.30	.14	.49
As	-.04	.09	.15	.02	-.01	-.17	-.19	-.17	.29	.15
S	-.13	.01	-.19	-.15	.22	.15	.06	-.01	-.11	.02
Cl	.17	-.26	-.14	-.03	.11	.30	-.27	-.44	.48	.32
Zr/Nb	-.42	.22	.06	-.03	.03	-.08	.49	.62	-.29	-.50
Ce/Y	.38	.38	-.47	.02	.24	.34	-.82	-.68	.05	.83

CORRELATION MATRIX

	P2O5	Ba	Rb	Sr	Pb	Th	U	Zr	Nb	Y
P2O5	1.00									
Ba	.69	1.00								
Rb	.47	.76	1.00							
Sr	-.02	-.01	-.33	1.00						
Pb	.52	.80	.95	-.29	1.00					
Th	.08	.43	.82	-.57	.73	1.00				
U	-.05	.13	.24	-.12	.26	.24	1.00			
Zr	.85	.74	.67	-.01	.71	.26	.09	1.00		
Nb	.60	.85	.68	.17	.73	.28	.20	.84	1.00	
Y	.83	.81	.74	-.15	.78	.38	.16	.97	.84	1.00
La	.68	.87	.88	-.10	.91	.56	.21	.86	.89	.90
Ce	.74	.85	.86	-.11	.90	.53	.19	.91	.88	.94
Nd	.85	.83	.77	-.07	.82	.39	.13	.96	.85	.97
Sc	.21	-.30	-.06	-.16	-.09	-.10	.15	.26	-.08	.17
V	-.41	-.68	-.26	-.19	-.30	-.12	.07	-.21	-.39	-.30
Cr	-.67	-.76	-.77	.06	-.79	-.52	.04	-.37	-.65	-.68
Ni	-.75	-.77	-.77	-.02	-.79	-.40	-.13	-.52	-.62	-.51
Cu	-.41	-.63	-.61	-.04	-.61	-.39	.03	-.54	-.65	-.58
Zn	.74	.78	.78	-.28	.80	.47	.08	.89	.82	.91
Ga	.23	.33	.44	.07	.50	.24	.24	.64	.63	.61
As	-.04	-.02	.19	.17	.11	.27	-.03	.10	.15	.05
S	.09	.05	-.06	.17	-.02	-.15	-.20	.04	.04	-.01
Cl	.17	.41	.13	.27	.13	-.08	-.08	.26	.45	.27
Zr/Nb	.08	-.44	-.47	-.17	-.49	-.33	-.24	-.22	-.65	-.25
Ce/Y	.44	.67	.87	-.11	.88	.66	.20	.66	.72	.67

CORRELATION MATRIX

	La	Ce	Nd	Sc	V	Cr	Ni	Cu	Zn	Ga
La	1.00									
Ce	.99	1.00								
Nd	.94	.97	1.00							
Sc	.00	.06	.12	1.00						
V	-.35	-.32	-.32	.64	1.00					
Cr	-.82	-.82	-.79	.18	.48	1.00				
Ni	-.90	-.91	-.92	-.20	.20	.69	1.00			
Cu	-.66	-.65	-.60	.19	.41	.69	.56	1.00		
Zn	.88	.92	.91	.11	-.20	-.73	-.84	-.57	1.00	
Ga	.60	.61	.57	.29	.22	-.25	-.63	-.39	.55	1.00
As	.17	.17	.08	.17	.08	-.24	-.15	-.32	.08	.21
S	.01	.00	.06	-.10	.06	-.04	-.09	-.01	.05	.02
Cl	.24	.24	.27	-.42	-.37	-.19	-.20	-.21	.32	.12
Zr/Nb	-.51	-.44	-.30	.30	.16	.35	.32	.51	-.36	-.38
Ce/Y	.90	.88	.77	-.01	-.14	-.82	-.75	-.58	.76	.54

CORRELATION MATRIX

	As	S	Cl	Zr/Nb	Ce/Y
As	1.00				
S	-.27	1.00			
Cl	-.25	.38	1.00		
Zr/Nb	-.24	-.10	-.51	1.00	
Ce/Y	.33	.01	.28	-.59	1.00

9. CLUSTER

Cluster analysis is a method of grouping or clustering unknown objects in which no assumptions are made about the data. There are two basic modes of classification - Q-mode, in which objects (commonly samples) are classified, and R-mode, in which attributes (i.e., observations, such as element concentrations, made on these objects) are classified.

The method starts with each object as an individual group and joins the most similar objects and groups together using a particular linkage method until a single group has been formed. The final grouping is shown by means of a dendrogram. The similarity between two objects is expressed numerically by a similarity measure. This program, which is partly based on Bonham-Carter (1967), gives a choice of two similarity measures, the correlation coefficient and the proportional similarity coefficient (also known as the cosine theta coefficient). There are also two possible linkage methods (in which an object is linked to a group if it has the highest similarity with the average similarity measure of the group) available. If the weighted-pair group average method is used, the new average value for the group is calculated as the mean of the similarity measure of the new object and the previous group average. If the unweighted average method is used, the new average similarity measure of the group is calculated by summing the individual similarity measures of all objects in the group and dividing by the number of objects in the group. Unlike the weighted method, this technique does not weight the group average in favour of the new object. Further details of the cluster analysis technique are given by Le Maitre (1982).

To run the program (which actually includes two parts, CLUSTA and DEND), type CLUSTER.

A Cluster analysis file (normally of the form ????.CLU) must be specified. Note that this file must be generated in the STATS program, which includes options to add arithmetic expressions, drop elements and samples, and select groups. The following options must then be specified:

1. Q-mode (default) or R-mode.

2. The similarity measure - correlation coefficient (default) or proportional similarity coefficient.

3. The linkage method - weighted-pair group method (default) or unweighted.

4. Highest value of similarity (i.e., the upper limit of the Y-axis: 0-1, 1.0 by default).

5. Lowest value of similarity (i.e., the lower limit of the Y-axis: 0-1, 0.0 by default).

Note that the calculations take a significant amount of time to carry out. 100 samples for 40 variables will take up to 15 minutes, depending on the PC. The input data, transformed data matrix, and dendrogram details can be printed out from a file CLUSTER.PRN if required. An example printout is given below.

CLUSTER PROGRAM BY B.F.BONHAM-CARTER, UNIV OF TORONTO

NUMBER OF SAMPLES = 7

NUMBER OF ELEMENTS = 37

FROM STATS PROGRAM

CLUSTERING BY THE WEIGHTED PAIR-GROUP METHOD

USING CORRELATION COEFFICIENT OF ASSOCIATION

FROM STATS PROGRAM

PRINTOUT OF DATA MATRIX

86286237		53.0000	1.5600	14.9700	1.8500	9.0000	.1600	5.6400	8.1100	3.2700	.6300	.2600	.0000
.0000	.0000	1.1800	245.0000	11.0000	495.0000	3.0000	.5000	.2500	83.0000	16.0000	19.0000		
12.0000	27.0000	17.0000	18.0000	112.0000	164.0000	63.0000	34.0000	114.0000	21.0000	.2500	1130.0000		
185.0000													
86285964		49.6000	2.1100	14.6300	3.2100	8.1000	.1600	5.9800	8.1000	3.4600	1.3500	.5000	.0000
.0000	.0000	2.4600	543.0000	25.0000	877.0000	7.0000	2.0000	.5000	136.0000	37.0000	22.0000		
24.0000	50.0000	32.0000	17.0000	113.0000	142.0000	75.0000	32.0000	129.0000	20.0000	.2500	1670.0000		
495.0000													
86285905		50.7000	1.7100	14.7600	2.5900	8.1600	.1500	5.2800	8.2700	3.1800	.7800	.3400	.6800
.1300	2.5300	.0000	330.0000	15.0000	571.0000	5.0000	.5000	.2500	100.0000	23.0000	20.0000		
14.0000	35.0000	20.0000	21.0000	119.0000	128.0000	50.0000	31.0000	118.0000	20.0000	1.0000	1930.0000		
265.0000													
86285860		48.9000	2.2800	14.4000	2.8700	8.4000	.1600	5.8300	7.5700	3.2600	1.8300	.5600	1.0700
.0400	2.2400	.0000	495.0000	40.0000	857.0000	24.0000	2.0000	.2500	157.0000	41.0000	22.0000		
22.0000	54.0000	32.0000	18.0000	112.0000	136.0000	67.0000	34.0000	164.0000	20.0000	1.0000	1140.0000		
1320.0000													
86285690		51.6000	1.6900	14.9800	3.8100	7.0300	.1600	5.5200	8.1700	3.3500	.7800	.3500	.0000
.0000	.0000	2.0500	313.0000	14.0000	530.0000	4.0000	.5000	.2500	96.0000	22.0000	20.0000		
17.0000	32.0000	19.0000	24.0000	125.0000	144.0000	57.0000	37.0000	111.0000	20.0000	.5000	1180.0000		
270.0000													
86285682		52.3000	1.7200	15.2000	2.6600	8.0300	.1500	5.4900	8.5100	3.4200	.8400	.3600	.0000
.0000	.0000	1.3100	354.0000	15.0000	627.0000	3.0000	1.0000	.5000	102.0000	22.0000	22.0000		
16.0000	35.0000	22.0000	19.0000	117.0000	116.0000	46.0000	28.0000	111.0000	19.0000	.2500	980.0000		
245.0000													
86285678		51.9000	1.7700	15.2000	1.8200	8.5800	.1500	5.3500	8.4800	3.3800	.8600	.3600	.0000
.0000	.0000	2.1600	364.0000	15.0000	628.0000	5.0000	.5000	1.0000	106.0000	22.0000	21.0000		
16.0000	37.0000	23.0000	19.0000	117.0000	122.0000	49.0000	31.0000	115.0000	20.0000	.2500	1190.0000		
270.0000													

VARIABLES TRANSFORMED TO PERCENT OF THEIR RANGE

PRINTOUT OF TRANSFORMED DATA MATRI

86286237			1.0000	.0000	.7125	.0151	1.0000	1.0000	.5143	.5745	.3214	.0000	.0000	.0000
	.0000	.0000	.4797	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000		
	.0000	.0000	.0000	.1429	.0000	1.0000	.5862	.6667	.0566	1.0000	.0000	.1579		
	.0000													
86285964			.1707	.7639	.2875	.6985	.5431	1.0000	1.0000	.5638	1.0000	.6000	.8000	.0000
	.0000	.0000	1.0000	1.0000	.4828	1.0000	.1905	1.0000	.3333	.7162	.8400	1.0000		
	1.0000	.8519	1.0000	.0000	.0769	.5417	1.0000	.4444	.3396	.5000	.0000	.7263		
	.2731													
86285905			.4390	.2083	.4500	.3869	.5736	.0000	.0000	.7447	.0000	.1250	.2667	.6355
	1.0000	1.0000	.0000	.2852	.1379	.1990	.0952	.0000	.0000	.2297	.2800	.3333		
	.1667	.2963	.2000	.5714	.5385	.2500	.1379	.3333	.1321	.5000	1.0000	1.0000		
	.0705													
86285860			.0000	1.0000	.0000	.5276	.6954	1.0000	.7857	.0000	.2857	1.0000	1.0000	1.0000
	.3077	.8854	.0000	.8389	1.0000	.9476	1.0000	1.0000	.0000	1.0000	1.0000	1.0000		
	.8333	1.0000	1.0000	.1429	.0000	.4167	.7241	.6667	1.0000	.5000	1.0000	.1684		
	1.0000													
86285690			.6585	.1806	.7250	1.0000	.0000	1.0000	.3429	.6383	.6071	.1250	.3000	.0000
	.0000	.0000	.8333	.2282	.1034	.2225	.0476	.0000	.0000	.1757	.2400	.3333		
	.4167	.1852	.1333	1.0000	1.0000	.5833	.3793	1.0000	.0000	.5000	.3333	.2105		
	.0749													
86285682			.8293	.2222	1.0000	.4221	.5076	.0000	.3000	1.0000	.8571	.1750	.3333	.0000
	.0000	.0000	.5325	.3658	.1379	.3455	.0000	.3333	.3333	.2568	.2400	1.0000		
	.3333	.2963	.3333	.2857	.3846	.0000	.0000	.0000	.0000	.0000	.0000	.0000		
	.0529													
86285678			.7317	.2917	1.0000	.0000	.7868	.0000	.1000	.9681	.7143	.1917	.3333	.0000
	.0000	.0000	.8780	.3993	.1379	.3482	.0952	.0000	1.0000	.3108	.2400	.6667		
	.3333	.3704	.4000	.2857	.3846	.1250	.1034	.3333	.0755	.5000	.0000	.2211		
	.0749													

FROM STATS PROGRAM

CLUSTERING BY THE WEIGHTED PAIR-GROUP METHOD

SAMPLE NUMBERS		LEVEL OF ASSOCIATION	CYCLE NUMBER
1	5	.8362	1
2	4	.9038	1
6	7	.9454	1
1	6	.7989	2
1	2	.7603	3
1	3	.7480	4

FROM STATS PROGRAM

ORDER OF SAMPLES FOR DENDROGRAM PLOT

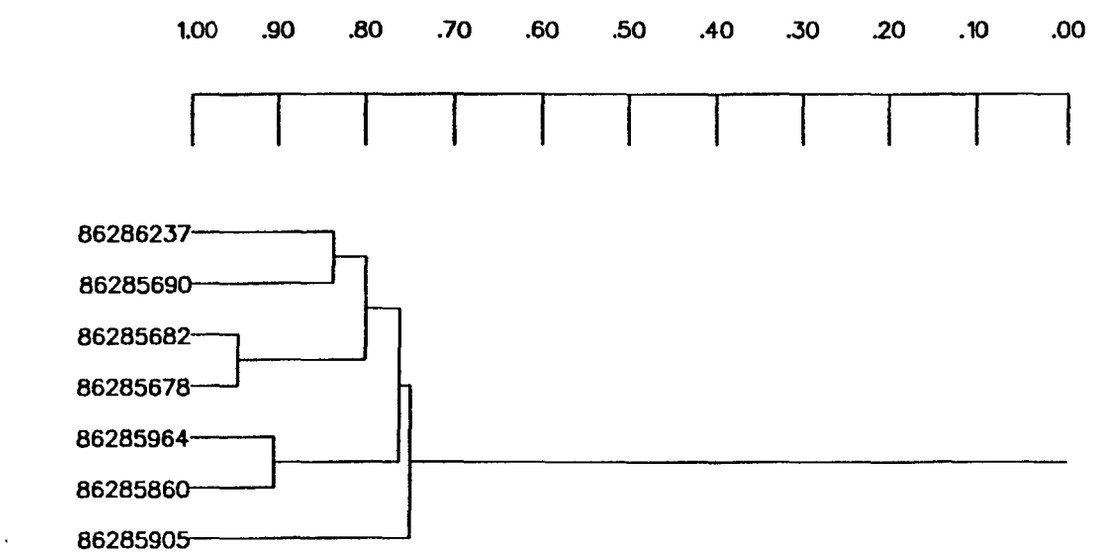
86286237	1
86285690	5
86285682	6
86285678	7
86285964	2
86285860	4
86285905	3

FROM STATS PROGRAM

INFORMATION REGARDING DENDROGRAM PLOT

LENGTH OF X-AXIS = 1. INCHES

Y-AXIS PLOTTED BETWEEN 1.0 AND .0



The dendrogram can be output either to the screen or to a metafile. To re-run the program to select a different output mode, it is only necessary to type DEND. The diagram is output as one or more separate plots, according to the number of samples included. Each part is treated as a separate metafile, but by outputting the first to the top left-hand quarter of the plotter page and the second to the bottom left, the two sections may be joined up. Three or more sections would require cutting and pasting.

Figure 9 gives two examples of dendrograms. Figure 9A is a Q-mode plot using the proportional similarity coefficient, and Figure 9B is the R-mode option with the similarity on the Y-axis set to 0.4 to 1.0.

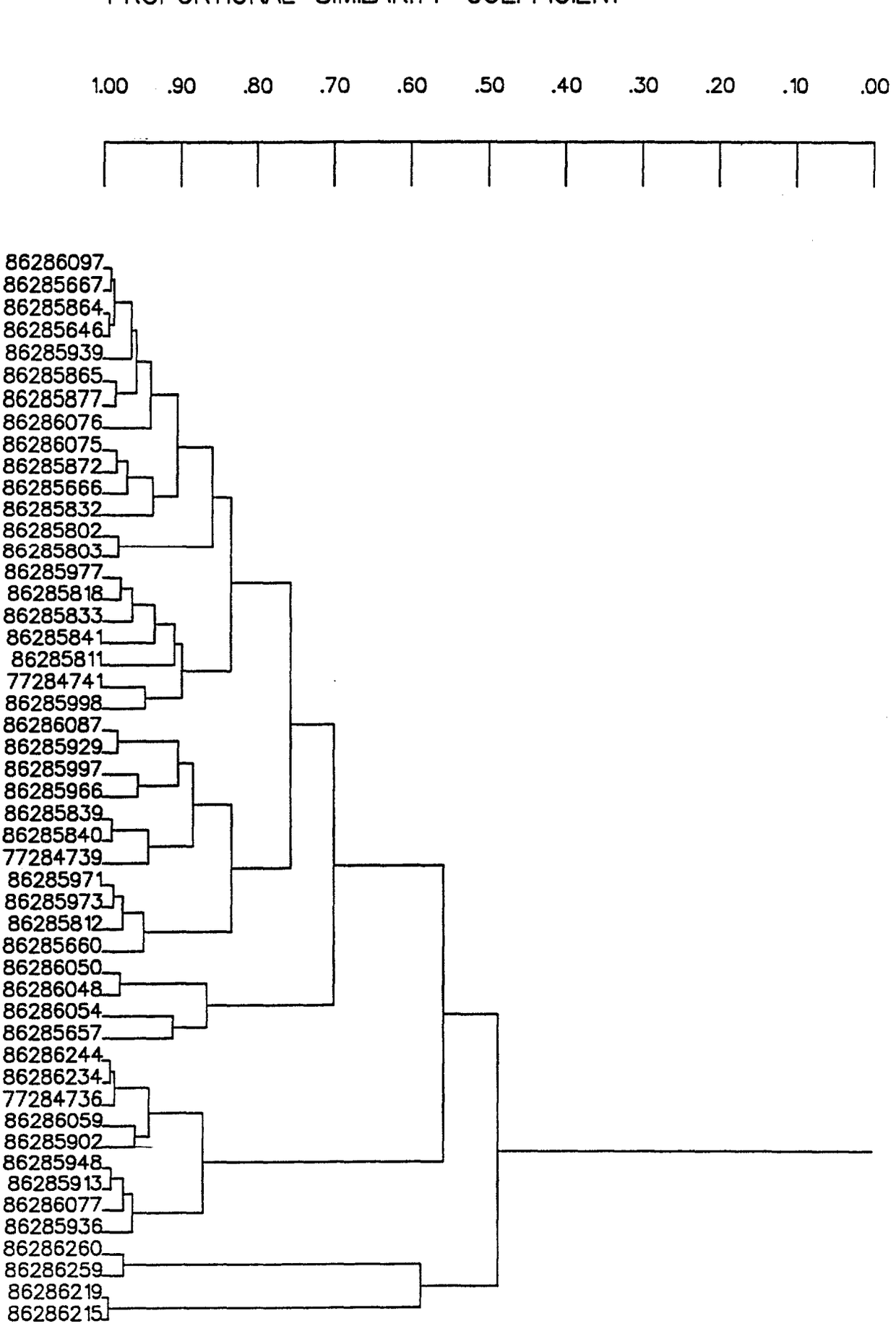

PROPORTIONAL SIMILARITY COEFFICIENT
1.00
.90
.80
.70
.60
.50
.40
.30
.20
.10
.00
86286097
86285667
86285864
86285646
86285939
86285865
86285877
86286076
86286075
86285872
86285666
86285832
86285802
86285803
86285977
86285818
86285833
86285841
86285811
77284741
86285998
86286087
86285929
86285997
86285966
86285839
86285840
77284739
86285971
86285973
86285812
86285660
86286050
86286048
86286054
86285657
86286244
86286234
77284736
86286059
86285902
86285948
86285913
86286077
86285936
86286260
86286259
86286219
86286215

FIG. 9A

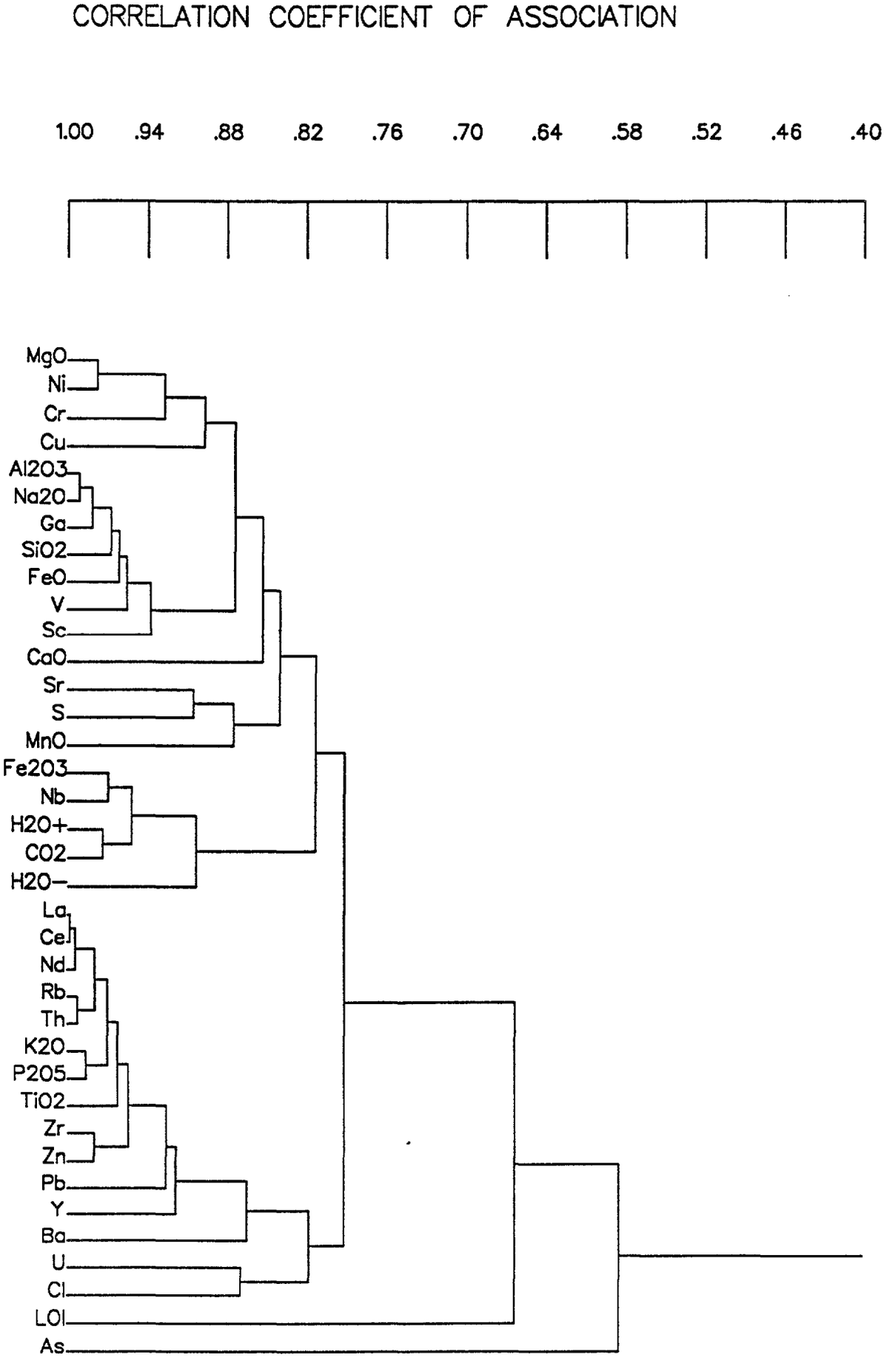

CORRELATION COEFFICIENT OF ASSOCIATION
1.00
.94
.88
.82
.76
.70
.64
.58
.52
.46
.40
MgO
Ni
Cr
Cu
Al2O3
Na2O
Ga
SiO2
FeO
V
Sc
CaO
Sr
S
MnO
Fe2O3
Nb
H2O+
CO2
H2O−
La
Ce
Nd
Rb
Th
K2O
P2O5
TiO2
Zr
Zn
Pb
Y
Ba
U
Cl
LOI
As

FIG. 9B

10. PETMOD

The petrogenetic modelling program, run by typing PETMOD, currently includes the following, although other models may be added later:

Equilibrium Batch Melting (using Henry's Law);
Rayleigh Fractional Crystallisation;
Major Element Fractionation;
Least-squares Mixing Calculations (PTMIX);
Incremental Olivine Addition.

The modelling definition file (MODEL.DEF) lists the major oxides and their default weightings for the least-squares mixing program:

```
Modelling definition file    MODEL.DEF
Oxides names and PTMIX wts
17
SiO2        2.0
TiO2         .5
Al2O3       2.0
Fe2O3       0.5
FeO         2.0
MnO          .2
MgO         2.0
CaO         2.0
Na2O        1.0
K2O         0.5
P2O5        0.5
Cr2O3       0.2
NiO         0.2
ZrO2        0.2
S           0.2
BaO         0.2
SrO         0.2
```

Mineral-melt distribution (i.e., partition) coefficient (Kd) data are given in files such as INTER.MEL (see Appendix C). For each model, results can be printed out from PETMOD.PRN.

10.1 EQUILBRIUM BATCH MELTING

This program uses the equilibrium batch melting equation, based on Henry's Law (Shaw, 1970):

$$\frac{C_L^e}{C_o^e} = \frac{1}{K_d^e + F(1-K_d^e)}$$

Where, e = trace element

C_o^e = initial concentration of element in source rock

C_L^e = concentration of element in partial melt

F= fraction of melting

K_d^e = bulk distribution coefficient for element e, given by

$$K_d^e = D_a^e A + D_b^e B + D_c^e C \ldots\ldots \text{ etc.}$$

where, D_a^e = distribution efficient for mineral a

A = fraction of mineral a in residue.

There are 3 options:

1. Calculation of element concentrations in the source rock (C_o^e) for a given analysed rock representing a partial melt (C_L^e).

2. Calculation of the melt fraction (F) given both source (C_o^e) and partial melt (C_L^e) compositions.

3. Calculation of element concentrations in the partial melt (C_L^e) formed from a given source composition (C_o^e).

In each case the residual mineralogy must be assumed, and 1 and 3 require the melt fraction (F) to be specified. Note that the sum of the weight fractions of the specified residual minerals must be 1. Distribution coefficients are normally read from a file, but different values may be substituted if required.

(1) Calculate element concentrations in source rock

This produces the following menu:

(1) Read mineral distribution coefficients off file (this should be done first, before selecting residual minerals, elements, etc.; INTER.MEL is the default).

(2) Change mineral distribution coefficient for an element and mineral (allows the above file to be edited before use).

(3) Select residual minerals (e.g., Ol, Cpx, Opx, Gt, Hb, Bi, Pl, Mt, Ap, Z).

(4) Select elements (e.g., Ti02, K20, Ba, Rb, Sr, Th, U, Zr, Nb, Y, La, Ce, Nd, Sc, V, Cr, Co, Ni, Zn).

(5) Specify weight fractions for selected minerals (note that the sum of these must = 1).

(6) Specify element concentrations in partial melt (for each selected element).

(7) Read partial melt concentrations off GDA file (instead of 6; the sample number must be specified).

(8) Specify melt fraction (between 0.0001 and 1.0).

(9) Display model result (on screen).

(10) Print model results (on file) (PETMOD.PRN).

(11) Display spidergram (the results may be displayed in the form of a spidergram to compare partial melt and model source; both may be normalised to primordial mantle abundances, or the partial melt may be normalised to the calculated source composition; the default file is SPIMOD.DEF, but others are available, e.g., REE.DEF for modelling rare-earth elements).

A table of the distribution coefficients for each selected element and residual mineral and weight fraction of each mineral, together with the assumed melt fraction, is displayed, followed by a table of the calculated concentration in the source and concentration in the partial melt for each selected element. If desired, different values of the mineral weight fractions, melt fraction and/or partial melt concentrations may be entered, and the calculations repeated.

(2) Calculate melt fraction

This differs from the first option in that element concentrations in both source rock and partial melt (either from keyboard or GDA file), rather than melt fraction, must be specified. Display of results is similar, except that the calculated melt fraction is given for each selected element. New element concentrations and/or mineral weight fractions may be entered, and the calculations repeated.

(3) Calculate element concentrations in partial melt

In this case the element concentrations in the source rock must be specified. Otherwise the data entry and display of results are similar to option 1.

The results of typical batch melting calculations are shown below.

EQUILIBRIUM BATCH MELTING

Mineral		Ol	Cpx	Opx
Weight fraction		.20	.50	.30
Dist. coeff.	TiO2	.0100	.3000	.1000
Dist. coeff.	K2O	.0070	.0200	.0100
Dist. coeff.	Ba	.0050	.0100	.0130
Dist. coeff.	Rb	.0100	.0200	.0100
Dist. coeff.	Sr	.0030	.1300	.0100
Dist. coeff.	Th	.0000	.0000	.0000
Dist. coeff.	U	.0000	.0000	.0000
Dist. coeff.	Zr	.0070	.1200	.0300
Dist. coeff.	Nb	.0060	.0200	.0200
Dist. coeff.	Y	.0020	.1950	.0090
Dist. coeff.	La	.0005	.0250	.0005
Dist. coeff.	Ce	.0008	.0400	.0009
Dist. coeff.	Nd	.0013	.0900	.0019
Dist. coeff.	Sc	.2500	3.10	1.20
Dist. coeff.	V	.0800	1.0000	.3000
Dist. coeff.	Cr	1.0000	7.00	3.00
Dist. coeff.	Co	3.80	1.20	1.40
Dist. coeff.	Ni	13.00	3.00	4.00
Dist. coeff.	Zn	2.13	.8200	2.60

Melt fraction .400

	TiO2	K2O	Ba	Rb	Sr	Th	U
Calc. conc. in source	1.02	.61	162.38	61.35	110.29	20.00	4.00
Conc. in liquid	2.00	1.50	400.00	150.00	250.00	50.00	10.00

	Zr	Nb	Y	La	Ce	Nd	Sc
Calc. conc. in source	110.56	8.21	13.81	18.34	35.04	17.10	39.40
Conc. in liquid	250.00	20.00	30.00	45.00	85.00	40.00	25.00

	V	Cr	Co	Ni	Zn
Calc. conc. in source	76.36	158.00	44.04	143.20	82.18
Conc. in liquid	100.00	50.00	30.00	40.00	60.00

EQUILIBRIUM BATCH MELTING

Mineral		Ol	Cpx	Opx
Weight fraction		.20	.50	.30
Dist. coeff.	TiO2	.0100	.3000	.1000
Dist. coeff.	K2O	.0070	.0200	.0100
Dist. coeff.	Ba	.0050	.0100	.0130
Dist. coeff.	Rb	.0100	.0200	.0100
Dist. coeff.	Sr	.0030	.1300	.0100
Dist. coeff.	Th	.0000	.0000	.0000
Dist. coeff.	U	.0000	.0000	.0000
Dist. coeff.	Zr	.0070	.1200	.0300
Dist. coeff.	Nb	.0060	.0200	.0200
Dist. coeff.	Y	.0020	.1950	.0090
Dist. coeff.	La	.0005	.0250	.0005
Dist. coeff.	Ce	.0008	.0400	.0009
Dist. coeff.	Nd	.0013	.0900	.0019
Dist. coeff.	Sc	.2500	3.10	1.20
Dist. coeff.	V	.0800	1.0000	.3000
Dist. coeff.	Cr	1.0000	7.00	3.00
Dist. coeff.	Co	3.80	1.20	1.40
Dist. coeff.	Ni	13.00	3.00	4.00
Dist. coeff.	Zn	2.13	.8200	2.60

	TiO2	K2O	Ba	Rb	Sr	Th	U
Conc. in source	1.00	.50	150.00	60.00	175.00	20.00	4.00
Conc. in liquid	2.00	1.50	400.00	150.00	250.00	50.00	10.00
Calc. melt fraction	.389	.324	.369	.391	.678	.400	.400

	Zr	Nb	Y	La	Ce	Nd	Sc
Conc. in source	125.00	10.00	20.00	20.00	45.00	25.00	45.00
Conc. in liquid	250.00	20.00	30.00	45.00	85.00	40.00	25.00
Calc. melt fraction	.462	.491	.629	.437	.520	.607	.167

	V	Cr	Co	Ni	Zn
Conc. in source	80.00	150.00	45.00	150.00	80.00
Conc. in liquid	100.00	50.00	30.00	40.00	60.00
Calc. melt fraction	.492	.389	.359	.360	.468

EQUILIBRIUM BATCH MELTING

Mineral		Ol	Cpx	Opx
Weight fraction		.20	.50	.30
Dist. coeff.	TiO2	.0100	.3000	.1000
Dist. coeff.	K2O	.0070	.0200	.0100
Dist. coeff.	Ba	.0050	.0100	.0130
Dist. coeff.	Rb	.0100	.0200	.0100
Dist. coeff.	Sr	.0030	.1300	.0100
Dist. coeff.	Th	.0000	.0000	.0000
Dist. coeff.	U	.0000	.0000	.0000
Dist. coeff.	Zr	.0070	.1200	.0300
Dist. coeff.	Nb	.0060	.0200	.0200
Dist. coeff.	Y	.0020	.1950	.0090
Dist. coeff.	La	.0005	.0250	.0005
Dist. coeff.	Ce	.0008	.0400	.0009
Dist. coeff.	Nd	.0013	.0900	.0019
Dist. coeff.	Sc	.2500	3.10	1.20
Dist. coeff.	V	.0800	1.0000	.3000
Dist. coeff.	Cr	1.0000	7.00	3.00
Dist. coeff.	Co	3.80	1.20	1.40
Dist. coeff.	Ni	13.00	3.00	4.00
Dist. coeff.	Zn	2.13	.8200	2.60

Melt fraction .400

	TiO2	K2O	Ba	Rb	Sr	Th	U
Conc. in source	1.00	.50	150.00	60.00	175.00	20.00	4.00
Calc. conc. in liquid	1.96	1.22	369.51	146.70	396.68	50.00	10.00

	Zr	Nb	Y	La	Ce	Nd	Sc
Conc. in source	125.00	10.00	20.00	20.00	45.00	25.00	45.00
Calc. conc. in liquid	282.65	24.37	43.44	49.06	109.15	58.48	28.55

	V	Cr	Co	Ni	Zn
Conc. in source	80.00	150.00	45.00	150.00	80.00
Calc. conc. in liquid	104.77	47.47	30.65	41.90	58.41

10.2 RAYLEIGH FRACTIONAL CRYSTALLISATION

This is analagous to the equilibrium batch melting model, but uses the Rayleigh non-equilibrium fractional crystallisation equation (Hanson, 1980):

$$\frac{C_L^e}{C_o^e} = F^{(K_d^e-1)}$$

where C_o^e = element concentration in parent magma
C_L^e = element concentration in residual liquid
F = fraction of residual liquid
K_d^e = bulk distribution coefficient for element e,
given by $K_d^e = D_a^e A + D_b^e B$...etc.
where, D_a^e = distribution coefficient for mineral a
A = fraction of mineral a in fractionating crystals.

There are three options:

(4) Calculation of element concentrations in the parent magma (C_o^e) for a given analysed rock representing a residual liquid (C_L^e).

(5) Calculation of the residual liquid fraction (F) given both parent magma (C_o^e) and residual liquid (C_L^e) compositions.

(6) Calculation of element concentrations in the residual liquid (C_L^e) derived by fractionation of a given parent magma (C_o^e).

In each case the fractionating phases must be assumed, and 4 and 6 require the fraction of residual liquid to be specified. Note that the sum of the weight fractions of the specified fractionating phases must be 1. Distribution coefficients are normally read off a file, but different values may be substituted if required.

(4) Calculate element concentrations in parent magma.

This produces the following menu:

(1) Read mineral distribution coefficients off file (should be done first).

(2) Change mineral distribution coefficients for an element and mineral.

(3) Select fractionating minerals.

(4) Select elements.

(5) Specify weight fractions for selected minerals (note that the sum of these must = 1).

(6) Specify element concentrations in residual liquid.

(7) Read residual liquid concentrations off GDA file.

(8) Specify fraction of residual liquid.

(9) Display model results.

(10) Print model results (on file) (PETMOD.PRN).

(11) Display spidergram (both model parent magma and residual liquid may be normalised to primordial mantle, or the residual liquid normalised to the calculated parent magma composition; the default file is SPIMOD.DEF - see Appendix C).

The display of results is similar to that for equilibrium batch melting, except that element concentrations in residual liquid and calculated parent magma are tabulated.

(5) Calculate residual liquid fraction.

Element concentrations in both parent magma and residual liquid are specified (either from keyboard or GDA file) and the residual liquid fraction calculated for each selected element.

(6) Calculate element concentrations in residual liquid.

In this case the element concentrations in the parent magma are specified. Otherwise the data entry and display of results are similar to option 4.

The results of a representative set of Rayleigh fractionation calculations, including examples of the optional spidergram output, are given below.

RAYLEIGH FRACTIONAL CYSTALLISATION

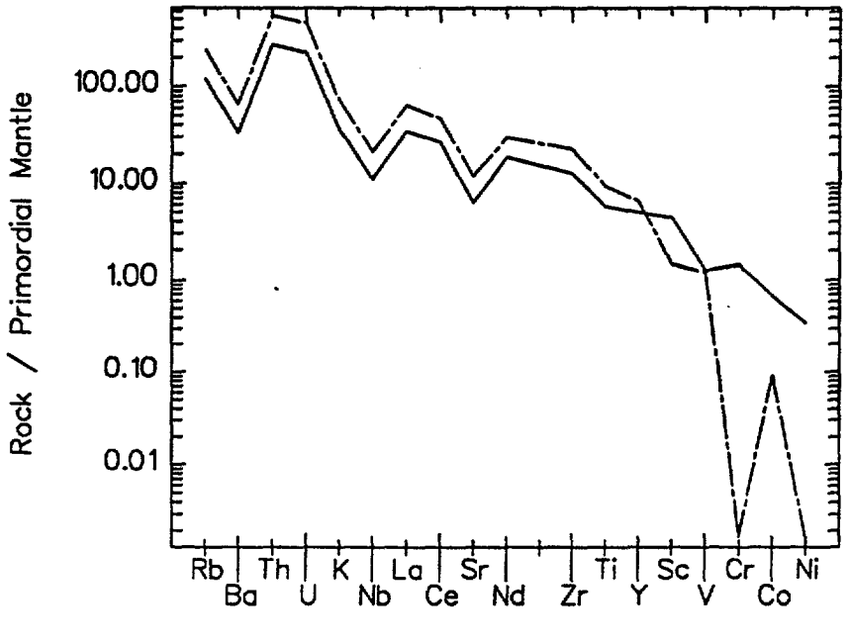
Mineral		Ol	Cpx	Opx
Weight fraction		.20	.50	.30
Dist. coeff.	TiO2	.0300	.4000	.2500
Dist. coeff.	K2O	.0100	.0200	.0100
Dist. coeff.	Ba	.0100	.0260	.0200
Dist. coeff.	Rb	.0100	.0300	.0100
Dist. coeff.	Sr	.0100	.1300	.0100
Dist. coeff.	Th	.0000	.0000	.0000
Dist. coeff.	U	.0000	.0000	.0000
Dist. coeff.	Zr	.0100	.2800	.0800
Dist. coeff.	Nb	.0100	.1000	.1000
Dist. coeff.	Y	.0200	1.03	.2800
Dist. coeff.	La	.0050	.1600	.0600
Dist. coeff.	Ce	.0080	.2700	.0800
Dist. coeff.	Nd	.0130	.6000	.1100
Dist. coeff.	Sc	.2800	3.30	3.00
Dist. coeff.	V	.0900	1.40	1.10
Dist. coeff.	Cr	1.15	15.00	10.00
Dist. coeff.	Co	5.50	2.00	6.00
Dist. coeff.	Ni	19.00	5.00	8.00
Dist. coeff.	Zn	2.11	6.00	3.50

Residual liquid fraction .500

	TiO2	K2O	Ba	Rb	Sr	Th	U
Calc. conc. in parent	1.22	1.01	228.30	76.05	131.21	25.00	5.00
Conc. in liquid	2.00	2.00	450.00	150.00	250.00	50.00	10.00

	Zr	Nb	Y	La	Ce	Nd	Sc
Calc. conc. in parent	140.24	7.94	22.78	24.10	47.50	25.24	76.10
Conc. in liquid	250.00	15.00	30.00	45.00	85.00	40.00	25.00

	V	Cr	Co	Ni	Zn
Calc. conc. in parent	103.38	4246.12	74.64	623.81	110.96
Conc. in liquid	100.00	5.00	10.00	3.00	10.00



RAYLEIGH FRACTIONAL CYSTALLISATION

Mineral		Ol	Cpx	Opx
Weight fraction		.20	.50	.30
Dist. coeff.	TiO2	.0300	.4000	.2500
Dist. coeff.	K2O	.0100	.0200	.0100
Dist. coeff.	Ba	.0100	.0260	.0200
Dist. coeff.	Rb	.0100	.0300	.0100
Dist. coeff.	Sr	.0100	.1300	.0100
Dist. coeff.	Th	.0000	.0000	.0000
Dist. coeff.	U	.0000	.0000	.0000
Dist. coeff.	Zr	.0100	.2800	.0800
Dist. coeff.	Nb	.0100	.1000	.1000
Dist. coeff.	Y	.0200	1.03	.2800
Dist. coeff.	La	.0050	.1600	.0600
Dist. coeff.	Ce	.0080	.2700	.0800
Dist. coeff.	Nd	.0130	.6000	.1100
Dist. coeff.	Sc	.2800	3.30	3.00
Dist. coeff.	V	.0900	1.40	1.10
Dist. coeff.	Cr	1.15	15.00	10.00
Dist. coeff.	Co	5.50	2.00	6.00
Dist. coeff.	Ni	19.00	5.00	8.00
Dist. coeff.	Zn	2.11	6.00	3.50

	TiO2	K2O	Ba	Rb	Sr	Th	U
Conc. in parent	1.00	1.00	200.00	70.00	150.00	20.00	5.00
Conc. in liquid	2.00	2.00	450.00	150.00	250.00	50.00	10.00
Calc. liquid fraction	.381	.495	.437	.459	.577	.400	.500

	Zr	Nb	Y	La	Ce	Nd	Sc
Conc. in parent	150.00	8.00	20.00	20.00	45.00	25.00	65.00
Conc. in liquid	250.00	15.00	30.00	45.00	85.00	40.00	25.00
Calc. liquid fraction	.542	.504	.360	.407	.469	.493	.552

	V	Cr	Co	Ni	Zn
Conc. in parent	105.00	4000.00	75.00	600.00	100.00
Conc. in liquid	100.00	5.00	10.00	3.00	10.00
Calc. liquid fraction	.362	.503	.499	.503	.515

RAYLEIGH FRACTIONAL CYSTALLISATION

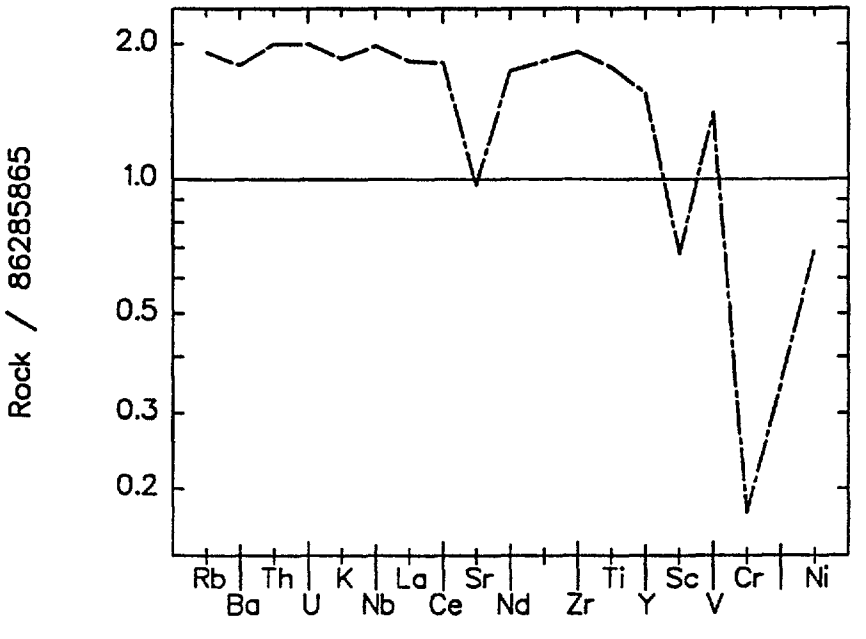
Mineral		Cpx	Pl
Weight fraction		.50	.50
Dist. coeff.	TiO2	.3000	.0400
Dist. coeff.	K2O	.0200	.2000
Dist. coeff.	Ba	.0100	.3000
Dist. coeff.	Rb	.0200	.1000
Dist. coeff.	Sr	.1000	2.00
Dist. coeff.	Th	.0000	.0000
Dist. coeff.	U	.0000	.0000
Dist. coeff.	Zr	.1000	.0100
Dist. coeff.	Nb	.0100	.0100
Dist. coeff.	Y	.6650	.0590
Dist. coeff.	La	.1100	.1400
Dist. coeff.	Ce	.1500	.1200
Dist. coeff.	Nd	.3100	.0810
Dist. coeff.	Sc	3.10	.0200
Dist. coeff.	V	1.0000	.0100
Dist. coeff.	Cr	7.00	.0200
Dist. coeff.	Ni	3.00	.0300
Dist. coeff.	Zn	.8200	.1000

Residual liquid fraction .500

	TiO2	K2O	Ba	Rb	Sr	Th	U
Conc. in parent	2.90	.82	290.00	16.00	307.00	1.00	.50
Calc. conc. in liquid	5.16	1.52	520.92	30.70	296.54	2.00	1.00

	Zr	Nb	Y	La	Ce	Nd	Sc
Conc. in parent	187.00	11.00	36.00	12.00	35.00	23.00	23.00
Calc. conc. in liquid	360.01	21.85	56.02	22.01	63.75	40.17	15.60

	V	Cr	Ni	Zn
Conc. in parent	200.00	65.00	105.00	111.00
Calc. conc. in liquid	281.86	11.41	73.48	161.39



10.3 MAJOR ELEMENT FRACTIONATION

The major element composition of a residual liquid (or partial melt) is calculated assuming fractionation of selected minerals from a given parent magma (or residual minerals remaining from a given source rock). The starting composition (parent magma or source rock) and fractionating (residual) mineral compositions and proportions are entered from the keyboard. The following mass balance equation is used:

$$C_L^e = \frac{C_o^e - PT}{1-P}$$

where, C_L^e = major element concentration in residual liquid (or partial melt)

C_o^e = major element concentration in parent magma (or source rock)

e = major element (oxide)

P = weight fraction of minerals in total (solid + melt) system

T = weight percent of major element in minerals.

For x minerals:

$$P = P_1 + P_2 + P_3 \ldots + P_x$$
$$PT = P_1T_1 + P_2T_2 + P_3T_3 \ldots + P_xT_x$$

The menu is as follows:

(1) Select major oxides.

(2) Specify fractionating (residual) minerals (enter a name, or abbreviation such as ol, opx).

(3) Specify major oxide concentrations in parent magma (source rock).

(4) Specify weight fractions of minerals in total (solid+melt) (for each specified mineral; total must be <1).

(5) Specify weight percent of each major oxide in each mineral.

(6) Display model results.

(7) Print model results (on file) (PETMOD.PRN).

(8) Print CIPW norm of residual liquid (or partial melt) (norm parameters must be specified - see GDA).

The parent magma, fractionating minerals and calculated residual liquid compositions, together with weight fractions of each mineral, are printed out. New values of the weight fractions may be entered and the calculation repeated if desired.

A typical set of results is given below.

Mineral	Parent magma	Residual liquid	Cpx	Plag
SiO2	50.70	50.31	50.92	51.00
TiO2	.61	1.19	.45	.00
Al2O3	14.80	11.53	3.56	30.40
Fe2O3	1.00	2.16	.00	.45
FeO	10.03	16.53	11.39	.00
MnO	.19	.30	.23	.00
MgO	8.13	8.61	15.62	.00
CaO	11.28	4.69	17.52	13.83
Na2O	1.79	1.32	.30	3.91
K2O	.14	.35	.00	.00
P2O5	.07	.18	.00	.00
Wt fraction			.30	.30

10.4 LEAST-SQUARES MIXING

This program calculates the proportions of a specified daughter product (residual liquid or partial melt) and specified mineral phases (fractionating or residual) derived from a specified parent composition (parent magma or source rock) by a least-squares fitting technique (Wright & Doherty, 1970).

The menu is:

(1) Select major oxides.

(2) Specify mixing mineral components (name or abbreviation, such as ol, opx, to a maximum of 10; the first is set to 'parent' and 'daughter' would normally be specified also).

(3) Specify percentage of each major oxide in each mineral.

(4) Specify mixing oxide weights (this allows different weightings to be assigned to each oxide; higher weights (say 2.0) would normally be assigned to the most important oxides (SiO_2, Al_2O_3, FeO, etc.), and lower weights (say 0.2) to the less important (MnO, Cr_2O_3, etc.); the default values are given on file MODEL.DEF).

(5) Specify whether addition or subtraction of components (normally +, but may be - for, say, cumulates).

(6) Drop a mixing mineral component (specify name).

(7) Add a mixing mineral component (specify name, and major oxide composition).

(8) Change percentage of major oxide in a mineral.

(9) Display model results.

(10) Print model results (on file) (PETMOD.PRN).

The printout of results includes the input data (parent, daughter and mineral compositions, and oxide weights), together with calculated proportions of daughter and specified minerals. The parent composition calculated from the latter is also given, with the differences from the actual (i.e., specified) parent and the sum of squares of these residuals (this is a measure of how good the 'fit' is).

An example of the table of results is given below. Note that in this case the sum of squares of the residuals is high (5.2145), showing that the fit is rather poor. Wright (1974) has argued that unless the residuals for all major oxides are less than 0.1% then the process postulated in the mixing model may not be correct.

INPUT DATA ACCEPTED

OXIDE	WEIGHT	Parent	+Daught	+Plag	+Cpx
SIO2	2.0	50.70	49.08	51.00	50.92
TIO2	.5	.61	2.55	.00	.45
AL2O3	2.0	14.80	12.22	30.40	3.56
FEO	2.0	11.13	18.32	.45	11.39
MNO	.2	.19	.28	.00	.23
MGO	2.0	8.13	4.77	.00	15.62
CAO	2.0	11.28	8.91	13.83	17.52
NA2O	1.0	1.79	2.47	3.91	.30
K2O	.5	.14	.61	.00	.00
P2O5	.5	.07	.32	.00	.00
TOTAL		98.84	99.53	99.59	99.99

SUM=1.0059, SOLUTIONS = .43151 .26583 .30858

CALCULATED DATA

OXIDE	WEIGHT	CALC	DIFF	Parent	Daught	Plag	Cpx
SIO2	2.0	50.45	-.251	50.70	49.08	51.00	50.92
TIO2	.5	1.24	.629	.61	2.55	.00	.45
AL2O3	2.0	14.45	-.347	14.80	12.22	30.40	3.56
FEO	2.0	11.54	.410	11.13	18.32	.45	11.39
MNO	.2	.19	.002	.19	.28	.00	.23
MGO	2.0	6.88	-1.252	8.13	4.77	.00	15.62
CAO	2.0	12.93	1.647	11.28	8.91	13.83	17.52
NA2O	1.0	2.20	.408	1.79	2.47	3.91	.30
K2O	.5	.26	.123	.14	.61	.00	.00
P2O5	.5	.14	.068	.07	.32	.00	.00
TOTAL		100.28		98.84	99.53	99.59	99.99
SOLUTIONS ARE		100.59%			43.15%	26.58%	30.86%
SENSITIVITY					.35	.40	.34

SUM OF SQUARES OF RESIDUALS = 5.2145

10.5 INCREMENTAL OLIVINE ADDITION

This program simulates olivine fractionation under conditions of surface equilibrium (Rayleigh fractionation). In particular, a primary magma composition can be estimated by incremental addition of olivine in equilibrium with a given mafic liquid (i.e., rock composition); after each addition the liquid composition is recalculated until a liquid in equilibrium with olivine of a peridotitic mantle source is obtained. Further details are given by Nicholls & Whitford (1976).

The menu is:

(1) Specify major oxide concentrations.

(2) Specify Fe-Mg distribution coefficient (for olivine, default = 0.30).

(3) Specify olivine increment (-2 to +2%).

(4) Specify number of increments (1-99; default = 20).

(5) Display model results.

(6) Print model results (on file) (PETMOD.PRN).

The starting and finishing compositions are displayed, together with the olivine mg value in each case, and the amount of olivine added (or subtracted). A typical printout is given below.

INCREMENTAL OLIVINE ADDITION

20 increments of 1.00%

	START	FINISH
SiO2	51.35	49.35
TiO2	.62	.51
Al2O3	14.99	12.29
Cr2O3	.01	.01
Fe2O3	1.01	.83
FeO	10.16	10.66
MnO	.19	.16
MgO	8.23	15.19
CaO	11.42	9.36
Na2O	1.81	1.48
K2O	.14	.11
P2O5	.07	.06
OL,MG	.828	.894

Olivine added= 18.0%

10.6 DEFINING PLOT PARAMETERS

Item 10 on the main PETMOD menu allows different plot parameters (although not linetypes, pen colours, or symbols) to be specified for the spidergram option in the equilibrium batch melting and Rayleigh fractional crystallisation programs. (See under GDA for further explanation).

11. UTIL

GDA files can be edited with the utilities program (UTIL). Although data held on a database such as ORACLE may be edited using the database facilities, it is sometimes convenient to use this program to merge files or add average analyses to a file. There are also facilities for creating new files, editing existing analyses, adding analyses, changing or adding field names, sorting samples on a file into numerical or element abundance order, deleting samples from a file and interrogating files.

The program is run by typing UTIL, and the starting menu is as follows:

(1) Create a new file (the fields on the new datafile are defined by a utilities field names file, such as the default UTIL.UTL; analyses may then be entered using option 5 below).

(2) Interrogate a file (descriptive and element fields, a list of sample numbers, and individual analyses may be displayed).

(3) Define new analysis on screen (for an existing GDA file; new sample number is specified, and new data (descriptive or element concentration) added; take care not to specify an existing sample number).

(4) Modify analysis on screen (for an existing GDA file; sample number is specified, and new data (descriptive or element concentration) added).

(5) Type in new analyses (for an existing GDA file; select fields (descriptive or element concentration) required, then enter data; take care not to specify an existing sample number).

(6) Type in values for a range of analyses (for an existing GDA file; select fields (descriptive or element concentration) required, specify first and last sample numbers for samples already on file (in file order), then enter new data for each).

(7) Modify an analysis (for an existing GDA file; give sample number, then new data).

(8) Sort file into analysis order (i.e., numerical order of sample numbers).

(9) Sort file into element abundance order (i.e., order of increasing abundance of any selected element).

(10) Merge another file, replacing values (if the second file has data fields that are not defined in the primary file, the primary file fields will be expanded to include them. Samples that are common to both files (same number) will cause values on the primary file to be replaced by those off the second file. New samples on the second file are added to the end of the primary file, but their order may be changed).

(11) Change a field name (change an existing field name).

(12) Add a field name (descriptive or element concentration; if the latter, samples must be re-assigned before any added data can be plotted; in either case, the report definition file (REPORT.RPT) will need to be edited).

(13) Write averages to a new file (sample numbers must be specified for each average - all samples, and each assigned group).

(14) Delete a range of analyses (first and last sample numbers must be specified, in the order they appear in the GDA file - not necessarily numerical order).

(15) Display structural formulae, normalise minerals (used with MDA program).

The default utilities field names file is UTIL.UTL, which includes all the standard GDA descriptive fields and elements. Other files include SPIDER.UTL for spidergrams and REE.UTL for rare-earth elements (see Appendix C). Other files can be set up (using the same format) if different descriptive and/or numerical fields are required. The numerical data fields do not necessarily need to contain element concentrations; any other data for plotting, such as isotopic ratios, could be entered.

12. OUTGDA

Analyses on a GDA file can be written to an ASCII file for further processing, e.g., entry into a database such as ORACLE. The names of both GDA and ASCII files must be given, and part of the file only may be output by specifying first and last sample numbers. The generated file has a header that gives the names of the fields (in alphabetical order), and the actual data follow.

A sample file is:

Data from file: john.gda
16 Description fields
AGE
BIBLIOREF
DEPTH
DRILLHOLE
GRIDREF
LITHOLOGY
LOCALITY
MAPNAME
MAPSYMBOL
ORIGINATOR
OTHERDATA
REGION
SAMPNO
STATE
STRATGROUP
STRATUNIT
58 Element concentrations
AG
AL2O3
AS
AU
B
BA
BE
BI
BR
C
CAO
CE
CL
CO
CO2
CR
CU
F
FE2O3
FEO
GA
GE
H2O+
H2O-
HG
K2O
LA
LI
LOI
MGO
MN
MNO
MO
NA2O
NB
ND
NI
P2O5
PB
RB
S
SC
SENTINAL
SIO2
SN

SR
TH
TIO2
U
V
W
XA
XB
XC
XD
Y
ZN
ZR
Protero
15,18

Bi-Op-QzPl gneiss
Filla Island

J. Sheraton
Rauer Op
Prydz Bay Coast
81285103
Antarctica

.000
16.500
-.500
.000
.000
905.000
2.000
.000
.000
.000
5.180
58.000
.000
.000
.000
53.000
19.000
.000
.780
4.660
22.000
.000
.540
.000
.000
1.210
28.000
22.000
.000
2.570
.000
.120
.000
4.080
19.000

34.000
26.000
.400
7.000
29.000
.000
17.000
1.C00
62.600
.000
506.000
1.000
1.060
-.500
90.000
.000
.000
.000
.000
.000
28.000
97.000
153.000
Protero
15,18

Gt-Pl-QzKf gneiss
Filla Island

J. Sheraton
Rauer Gt
Prydz Bay Coast
81285104
Antarctica

.000
13.610
-.500
.000
.000
800.000
2.000
.000
.000
.000
1.540
32.000
.000
.000
.000
6.000
4.000
.000
.440
1.170
15.000
.000
.360
.000
.000

```
      4.130
     18.000
     13.000
       .000
       .350
       .000
       .040
       .000
      3.870
      7.000
     16.000
      2.000
       .100
     25.000
     79.000
       .000
      2.000
      1.000
     74.200
       .000
    161.000
     12.000
       .130
      1.000
      8.000
       .000
       .000
       .000
       .000
       .000
     12.000
     36.000
     95.000
FINISH
```

13. SUMMARY

1. The first step in using the GDA system is to get analytical data in the form of datafiles (GDA files) suitable for processing. There are two ways of doing this. Data from a database such as ORACLE can be entered into the system on ASCII Files. Such files are transferred to GDA files using the ORACLE program. Alternativerly, data may be entered directly from the keyboard onto GDA files using the utilities program (UTIL). A new file must be created, and data are then entered into specified descriptive or element fields. The UTIL program program may also be used to edit or merge existing GDA files.

2. Before GDA files can be used, samples must be assigned to one or more groups using the ASSIGN program. This is done by specifying logical conditions for each group, such as a particular locality, lithology, or age. Samples in a group are plotted with the same symbol and colour. It is recommended that the logic is stored on a file for subsequent re-use and/or editing.

3. Once samples have been assigned to groups, data on GDA files can be used in the various data-processing programs (GDA, PLOT, TABLE, STATS, CLUSTER, and PETMOD).

4. The main processing programs (GDA, and the version for 1000-2000 samples, BIGGDA) are used to generate plots, initially on the PC screen, and then as plot metafiles for output to plotters. Firstly, data (element concentrations, arithmetic expressions such as ratios, or CIPW normative minerals) are extracted into datasets. Secondly, the selected datasets are used to produce histograms, XY plots, triangular plots, or spidergrams. Finally, the required plots are written to metafiles for subsequent output to plotters. Additional facilities in the program are calculation of CIPW norms and statistical functions, and selection of plotting parameters (symbol and text sizes and colours, plot axis lengths, etc). The latter can be stored on a file for subsequent re-use.

5. Output of plot metafiles to plotters is carried out by the PLOT program. Plots may either be output directly from metafiles to a

connected plotter, or written to HPGL files for output to an offline plotter or laser printer. There are facilities for positioning plots on a page, and for outputting a number of plots on a single page.

6. TABLE allows printing of tables of major and trace element data, CIPW norms, and element ratios or other expressions. One or more groups may be selected, and the number of samples per page may be specified.

7. The STATS program is used to calculate statistical functions, comprising mean, standard deviation, maximum, minimum, and an optional correlation matrix. It is also used to generate the input file for the CLUSTER program. One or more groups may be selected for the calculations.

8. CLUSTER is a Q- or R-mode cluster analysis program with dendrogram output. It requires an input datafile generated in the STATS program.

9. Various petrogenetic modelling programs are included in PETMOD. This presently contains equilibrium batch melting, Rayleigh fractional crystallisation, major element fractionation, least-squares mixing calculations, and incremental olivine addition options. In each case, results can either be displayed on the screen, or output to files for subsequent printing.

10. A program OUTGDA can be used to write analyses from GDA to ASCII files for input to other systems or databases.

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APPENDIX A. RESTRICTIONS

There are limits on the capacity of the software due to the limits imposed by the MS-DOS operating system, HALO graphics package and design decisions.

Max	Description
50	number of groups
11	number of datasets (standard)
4	number of datasets (BIGGDA,MDA)
1000	number of assigned samples (GDA,MDA)
2000	" " " " (BIGGDA)
15	number of symbols
8	number of plotter pens
3	number of linetypes
10	number of logic lines to specify a group
25	number of descriptive fields in GDA file
100	number of element concentrations in GDA file
40	number of element ratios in a spidergram
100	number of bars in a histogram
20	number of sample numbers typed in for spidergram
5	number of additional points for plots
10	number of columns in report
1000	number of samples for least squares line fit
0	number of samples for least squares line fit (BIGGDA,MDA)
15	number of minerals for modelling
10	number of least squares mixing minerals
12	number of olivine addition oxides
5000	number of samples in a GDA file that can be sorted or merged by the UTIL program
250	number of samples or variables in CLUSTER program
25	number of characters of text for added plot points or text
20	number of additional plot points and/or text lines.

APPENDIX B. SOFTWARE MAINTENANCE

Most software files are held on directory \gda\ with the HALO system on \halo\ . The directory \biggda\ is used for building the larger capacity gda program BIGGDA, and \mingda\ for the minerals program MDA (when available).

The programs use software simulation of floating point operations so they will run on most PCs. The software is written in FORTRAN 77 (Microsoft compiler) and consists of over 20 000 lines of source code. The exception is the arithmetic calculator routine ARITH.IFT, which is written in a higher level language IFTRAN. This code must be run through the IFT preprocessor to produce the FORTRAN source code. If the system is transported to another computer the FORTRAN source ARITH.FOR can be used directly, although it is not very readable. There has not been enough time to convert the routine to standard FORTRAN.

The whole system can be built by typing 'all' in directory \gda\ .

Each program has a file (with extension .LNK) that is used for linking. Some programs have a simple overlay structure. All COMMON blocks and major arrays are on files (with extension .INS) and are inserted by the compiler into the source code.
Changing a system limit requires modifying array definitions in the insert files, changing the limit definition in GDABLK.FOR and typing 'all' to rebuild. The second directory \biggda\ holds a second set of definitions for the version of the program that allows larger numbers of samples to be handled, and a version of GDABLK.FOR that defines the limits.
Similarly, the \mingda\ directory has insert files for the MDA program.

Least squares line fitting was dropped from BIGGDA and MDA to gain more space.

Once the system has been compiled the command file RELEASE.BAT can be used to copy all the necessary files to ten 360k floppies for installation of the system on other PCs (see INSTALLATION). A similar file RELMIN.BAT is used for the minerals programs.

The source code (FORTRAN) files on each directory can be copied to floppy disks with the command file BACKUP.

The command file CLEANUP.BAT removes surplus files from the gda directory.

Support for graphics is provided by the HALO package. The system expects to generate graphics either directly on the screen or to a metafile. The HALO package provides translators to output the metacode to HP plotters or to files of HPGL commands. This code is relatively independent of HALO and if the module PLTSUB.FOR were rewritten, other graphics packages could be used.

The source code can be installed on an IBM PC as follows:

. Install Microsoft FORTRAN;
. Copy the HALO files for Microsoft FORTRAN to halo ;
. Copy from halo into gda ;
. The appropriate plotter translator file(s) which should be renamed, e.g., copy halo HALO7550.EXE HP7550.EXE

  All *.FNT files (fonts)

  The appropriate screen graphics driver, which should be renamed as SCREEN.DEV (e.g., copy halo HALOIBME.DEV SCREEN.DEV);

. [If a co-processor is available, the FL commands in ALL.BAT will have to be edited (to remove /FPi);]

. Copy the Source Code floppies to gda , biggda , and, if appropriate, mingda ;

. Type 'all' under gda.

The whole system takes over 2 hours to build up, and once built, all HALO and FORTRAN directory files can be deleted.

APPENDIX C. PARAMETER FILES

Various types of parameter file are available for use in entering data or expressions, defining spidergram plots, storing distribution coefficients, etc. New files may be set up as required, provided the format of the given file type is adhered to.

STDEXP.DEF and STDSET.DEF contain arithmetic expressions and standard datasets for use in extracting data in the GDA program. Details of the various triangular plots used for metamorphic rocks are given in Winkler (1974).

Spidergram plot definition files are used to specify the elements, element order, and normalising values for spidergram plots:

SPIDER.DEF is for standard spidergrams;
ARACH.DEF is similar, but Pb is placed after Ce for mafic rocks;
REE.DEF is for rare-earth plots (note blank for Pm);
SPIMOD.DEF is primarily for use with the PETMOD programs.

Chondritic normalising values (Nakamura, 1974, Evensen & others, 1978) are used for rare-earth element plots, whereas estimated primordial mantle abundances (McDonough, 1987) are used for the other spidergrams. The normalising value for Pb used in ARACH.DEF is considered to be a more realistic estimate of the primordial mantle abundance (= Ce/25: S-S. Sun, personal communication, 1988).

The utilities program (UTIL) uses utilities field name files to define the descriptive and element concentration fields for new GDA files. This enables data for only the elements of interest to be entered:

UTIL.UTL is for standard GDA files;
SPIDER.UTL is for spidergrams;
REE.UTL is for rare-earth elements.

Distribution (partition) coefficients (Kd) are stored in files such as INTER.MEL, which contains Kd values for melting of intermediate rocks. Other files can be set up for mafic (MAFIC.) or felsic (FELSIC.) rocks,

crystal fractionation models (.XL), or rare-earth elements (e.g., INTREE.). At present, only one set of Kd files (.MEL) has been compiled for use with both melting and fractional crystallisation modelling programs. This is because of the lack of reliable Kd data for many elements. However, the programs allow any of the Kd values to be changed before use. Sources of data for rare-earth elements comprise Arth (1976), Frey & others (1978), Mahood & Hildreth (1983), Henderson (1984), Fujimaki (1986), Green & Pearson (1986), and A. Ewart (unpublished data). Data for other elements were compiled from Arth (1976), Allègre & others (1977), Schock (1977, 1979), Irving (1978), Frey & others (1978), Gill (1978, 1981), McCallum & Charette (1978), Pearce & Norry (1979), Luhr & Carmichael (1980), Villemant & others (1981), Clague & Frey (1982), Ewart (1982, unpublished data), Mahood & Hildreth (1983), Fujimaki (1986), Lemarchand & others (1987), Schearer & others (1987), and Green & others (1988).

To avoid confusion, it is recommended that any new files are named according to the nomenclature given above. Thus, spidergram plot definition files should end in .DEF, utilities files in .UTL, etc.

```
STDEXP.DEF
Standard Arithmetic Expressions
(Al2O3/101.94)/(CaO/56.08-P2O5/42.59+Na2O/61.98+K2O/94.2)
ASI
(100*MgO/40.32) / (FeO/71.85+MGO/40.32)
mg
(100*MgO/40.32) / (FeO/71.85+Fe2O3/79.85+MgO/40.32)
mg
(100*MgO/40.32) /( # * (FeO+0.9*Fe2O3)/71.85+MgO/40.32)
mg
Na2O + K2O
Na2O+K2O
FeO + 0.8998*Fe2O3
Total Fe as FeO
0.9*Fe2O3 / (0.9*Fe2O3+FeO)
Fe3/(Fe2+Fe3)
(K2O/94.2)/(Na2O/61.98+K2O/94.2)
k
8301*K2O/Rb
K/Rb
Ga / (0.5291*Al2O3)
10000Ga/Al
2.5*Ce/Y
(Ce/Y)n
Sr/(5.77*Ce+7.74*Nd)
Sr/Sr*
Nb/(12.82*K2O+0.507*La)
Nb/Nb*
CaO-1.3168*P2O5+1.8096*Na2O+1.1907*K2O
C
0.561*FeO+0.5682*MnO+MgO-0.5045*TiO2
M
Al2O3+0.000098*Cr+0.6384*Fe2O3+1.645*Na2O+1.0824*K2O+1.2761*TiO2
A
SiO2-1.939*Na2O-1.2758*K2O
S
```

STDSET.DEF

```
Standard Dataset Definitions
Major Elements
11
SiO2
TiO2
Al2O3
Total Fe as FeO
MgO
CaO
Na2O
K2O
Na2O+K2O
P2O5
ASI
SiO2
TiO2
Al2O3
FeO + 0.8998*Fe2O3
MgO
CaO
Na2O
K2O
Na2O+K2O
P2O5
(Al2O3/101.94)/(CaO/56.08-P2O5/42.59+Na2O/61.98+K2O/94.2)
Trace Elements
11
SiO2
Ba
Rb
Sr
Th
Zr
Nb
Y
Ce
Cr
Ni
SiO2
Ba
Rb
Sr
Th
Zr
Nb
Y
Ce
Cr
Ni
Igneous AFM (Weight %)
03
K2O+Na2O
Total FeO
MgO
NA2O+K2O
FeO+0.9*Fe2O3
MGO
Igneous ACF (Molecular %)
```

```
03
CaO
Al2O3-K2O-Na2O
FeO+MgO
CAO/56.08
AL2O3/101.94-NA2O/61.98-K2O/94.2
MGO/40.32+FEO/71.85
Ti-Zr-Y (Pearce & Cann, 1973)
03
Zr
Ti/100
Y * 3
Zr
TIO2*59.95
Y*3.0
Ti-Mn-P (Mullen, 1983)
03
MnO*10
TiO2
P2O5*10
MNO * 10.0
TIO2
P2O5*10.0
Nb-Zr-Y (Meschede,1986)
03
Zr/4
Nb*2
Y
Zr/4
Nb*2
Y
Metamorphic A'KF ( Molecular % ;Uncorrected)
03
F
A'
K
MgO/40.32+MnO/70.94+FeO/71.85
AL2O3/101.94+FE2O3/159.7-NA2O/61.982-K2O/94.2-CaO/56.08
K2O/94.2
Metamorphic ACF ( Molecular % ;Uncorrected)
03
C
A
F
CaO/56.08-P2O5/42.59
Al2O3/101.94+Fe2O3/159.7-Na2O/61.98-K2O/94.2
MgO/40.32+MnO/70.94+FeO/71.85
Metamorphic A'FM (+Qtz,Ksp,Plag,Mt,Il)
03
F
A'
M
FeO/71.85-Fe2O3/159.7-TiO2/79.9
Al2O3/101.94-K2O/94.2-Na2O/61.98-CaO/56.08
MgO/40.32
Metamorphic SFA'
03
F
```

```
S
A'
FeO/71.85+Fe2O3/79.85+MgO/40.32
SiO2/60.09-K2O/15.7-Na2O/10.33-CaO/28.04
Al2O3/101.94-K2O/94.2-Na2O/61.98-CaO/56.08
Metamorphic AFM (+quartz,muscovite; uncorrected)
06
F Use set 4
A Use set 5
M Use set 6
F
A
M
(FeO/71.85)/(Mgo/40.32+FeO/71.85)
(Al2O3/101.94-K2O/31.4)/(Al2O3/101.94-K2O/31.4+FeO/71.85+MgO/40.32)
(MgO/40.32) / (FeO/71.85+MgO/40.32)
100.0 * $1 * (1.0 - $2)
100.0 * $2
100.0 * $3 * (1.0 - $2)
Metamorphic AFM (+quartz,K-feldspar; uncorrected)
06
F Use set 4
A Use set 5
M Use set 6
F
A
M
(FeO/71.85)/(Mgo/40.32+FeO/71.85)
(Al2O3/101.94-K2O/94.2)/(Al2O3/101.94-K2O/94.2+FeO/71.85+MgO/40.32
(MgO/40.32) / (FeO/71.85+MgO/40.32)
100.0 * $1 * (1.0 - $2)
100.0 * $2
100.0 * $3 * (1.0 - $2)
```

```
SPIDER.DEF
Spidergram Plot Definition File
Rock / Primordial Mantle
Pb
Pb / 0.20
Rb
RB / 0.63
Ba
BA /6.91
Th
TH / 0.092
U
U / 0.022
K
K2O / 0.0277
Nb
NB / 0.71
La
LA / 0.70
Ce
CE / 1.81
Sr
SR / 20.9
Nd
ND / 1.35
P
P2O5 / 0.0218
Zr
ZR / 11.1
Ti
TIO2 / 0.2118
Y
Y / 4.52
Na
NA2O / 0.3895
```

```
ARACH.DEF
Spidergram Plot Definition File
Rock / Primordial Mantle
Rb
RB / 0.63
Ba
BA /6.91
Th
TH / 0.092
U
U / 0.022
K
K2O / 0.0277
Nb
NB / 0.71
La
LA / 0.70
Ce
CE / 1.81
Pb
Pb / 0.0724
Sr
SR / 20.9
Nd
ND / 1.35
P
P2O5 / 0.0218
Zr
ZR / 11.1
Ti
TIO2 / 0.2118
Y
Y / 4.52
Na
NA2O / 0.3895
```

```
REE.DEF
Spidergram Plot Definition File
Rock / Chondrite
La
LA / 0.329
Ce
CE / 0.865
Pr
PR / 0.128
Nd
Nd / 0.630
Pm

Sm
SM / 0.203
Eu
EU / 0.077
Gd
GD / 0.276
Tb
TB / 0.0498
Dy
DY / 0.343
Ho
HO / 0.0754
Er
Er / 0.225
Tm
TM / 0.0341
Yb
Yb / 0.220
Lu
Lu / 0.0339
```

```
SPIMOD.DEF
Spidergram Plot Definition File
Rock / Primordial Mantle
Rb
RB / 0.63
Ba
BA /6.91
Th
TH / 0.092
U
U / 0.022
K
K2O / 0.0277
Nb
NB / 0.71
La
LA / 0.70
Ce
CE / 1.81
Sr
SR / 20.9
Nd
ND / 1.35
P
P2O5 / 0.0218
Zr
ZR / 11.1
Ti
TIO2 / 0.2118
Y
Y / 4.52
V
V / 82.0
Sc
SC / 17.1
Cr
CR / 2915.0
Co
CO / 110.0
Ni
NI / 1800.0
```

Utilities field names file UTIL.UTL
Description Fields
SAMPNO
STATE
REGION
LOCALITY
STRATGROUP
STRATUNIT
MAPSYMBOL
LITHOLOGY
MAPNAME
GRIDREF
DRILLHOLE
DEPTH
AGE
BIBLIOREF
ORIGINATOR
OTHERDATA
Element Fields
SIO2
TIO2
AL2O3
FE2O3
FEO
MNO
MGO
CAO
NA2O
K2O
P2O5
H2O+
H2O-
CO2
LOI
BA
LI
RB
SR
PB
TH
U
ZR
NB
Y
LA
CE
ND
PR
SC
V
CR
MN
CO
NI
CU
ZN
SN
W
MO
GA
AS
S
C
F

CL
BE
B
AG
AU
HG
BI
SB
HF
TA
CS
GE
BR
SE
PT
PD
IR

Utilities field names file SPIDER.UTL
Description Fields
SAMPNO
Element Fields
TIO2
NA2O
K2O
P2O5
BA
RB
SR
PB
TH
U
ZR
NB
Y
LA
CE
ND

Utilities field names file REE.UTL
Description Fields
SAMPNO
Element Fields
La
Ce
Pr
Nd
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu

Distribution coefficients MAFIC.MEL - Mafic rocks

	Ol	Cpx	Opx	Gt	Hb	Bi	Pl	Mt	Il	Ap	Sp
TiO2	0.01	0.3	0.1	0.3	2.0	1.5	0.04	7.5			0.8
K2O	0.007	0.02	0.01	0.01	0.7		0.20				
Ba	0.005	0.01	0.013	0.02	0.45	2.0	0.30				
Rb	0.01	0.02	0.01	0.02	0.25	2.5	0.10				
Sr	0.003	0.10	0.02	0.02	0.35	0.24	2.0			1.0	
Th	0.0	0.0	0.0	0.0	0.11	0.08	0.0			5.2	
U	0.0	0.0	0.0	0.0	0.15	0.08	0.0			4.0	
Zr	0.007	0.10	0.10	0.5	0.5	0.6	0.01	0.1	0.33	0.43	0.55
Nb	0.006	0.01	0.02	0.02	0.8	1.0	0.01	0.4	0.81		
Y	0.002	0.665	0.009	1.083	0.6	0.032	0.059	0.017	0.130	9.6	0.108
La	0.0005	0.11	0.0005	0.002	0.14	0.035	0.14	0.015	0.098	9.3	0.032
Ce	0.0008	0.15	0.0009	0.0033	0.20	0.034	0.12	0.016	0.110	9.6	0.033
Nd	0.0013	0.31	0.0019	0.0184	0.33	0.032	0.081	0.023	0.140	10.0	0.038
Sc	0.25	3.1	1.2	6.5	3.0	10.0	0.02	2.0	1.8		0.1
V	0.08	1.0	0.3	2.1	2.0	10.0	0.01	17.0	12.0		38.0
Cr	1.0	7.0	3.0	10.0	3.4	12.0	0.02	10.0	6.0		350.0
Co	3.8	1.2	1.4	2.0	2.7	26.0	0.05	6.0	2.6		10.0
Ni	13.0	3.0	4.0	0.8	2.0	1.3	0.03	12.0	12.0		11.0
Zn	2.13	0.82	2.6	1.0	6.8	3.0	0.10	11.9	0.38		

Distribution coefficients INTER.MEL - Intermediate rocks

	Ol	Cpx	Opx	Gt	Hb	Bi	Pl	Ksp	Mt	Il	Ap	Z
TiO2	0.03	0.4	0.25	0.5	3.0	1.5	0.05	0.05	9.0			
K2O	0.01	0.02	0.01	0.01	0.33		0.18					
Ba	0.01	0.026	0.02	0.02	0.15	6.2	0.30	3.8				
Rb	0.01	0.03	0.01	0.01	0.05	3.0	0.05	0.4				
Sr	0.01	0.13	0.01	0.02	0.23	0.12	2.4	3.0			2.0	
Th	0.0	0.0	0.0	0.0	0.11	0.3	0.0	0.05			5.2	28.0
U	0.0	0.0	0.0	0.0	0.15	0.1	0.0	0.06			4.0	66.0
Zr	0.01	0.28	0.10	0.5	0.9	1.2	0.02	0.003	0.3	0.5	0.77	
Nb	0.01	0.10	0.10	0.05	1.3	1.8	0.02	0.004	1.0	2.0		
Y	0.02	1.03	0.28	35.7	6.07	0.175	0.042	0.006	0.341	1.11	13.8	45.0
La	0.005	0.16	0.06	0.26	0.44	0.18	0.212	0.053	0.247	1.85	10.0	0.28
Ce	0.008	0.27	0.08	0.35	0.90	0.18	0.150	0.044	0.291	1.78	12.0	0.27
Nd	0.013	0.60	0.11	0.53	2.80	0.16	0.108	0.025	0.396	1.67	16.0	0.26
Sc	0.28	3.3	3.0	10.0	10.0	13.0	0.02	0.07	3.0	1.8		
V	0.09	1.4	1.1	8.0	10.0	50.0	0.02	0.55	28.0	20.0		
Cr	1.15	15.0	10.0	20.0	30.0	5.0	0.03	0.56	10.0	6.0		
Co	5.5	2.0	6.0	2.0	13.0	25.0	0.02	0.55	6.7	2.2		
Ni	19.0	5.0	8.0	0.6	10.0	13.0	0.05	1.1	10.0	10.0		
Zn	2.11	6.0	3.5	6.0	6.8	9.0	0.07	0.1	11.9	1.2		

Distribution coefficients FELSIC.MEL - Felsic rocks

	Ol	Cpx	Opx	Gt	Hb	Bi	Pl	Ksp	Mt	Il	Ap	Z	Sph	All
TiO2	0.03	0.7	0.40	1.2	7.0	2.5	0.05		12.5					
K2O	0.01	0.037	0.01	0.01	0.08		0.15							
Ba	0.01	0.05	0.03	0.02	0.044	6.2	0.9	7.0						
Rb	0.015	0.03	0.01	0.01	0.014	3.0	0.05	0.8						
Sr	0.04	0.33	0.01	0.015	0.022	0.10	6.0	3.9			10.0			
Th	0.0	0.0	0.0	0.22	0.11	0.5	0.0	0.02			1.1	30.0		200
U	0.0	0.0	0.0	0.40	0.15	0.1	0.0	0.02			2.9	100.0		15.
Zr	0.01	0.67	0.20	1.2	4.0	2.0	0.10	0.01	0.7	1.0	2.6			
Nb	0.01	0.20	0.20	0.1	4.0	3.0	0.03	0.006	2.5	4.0		4.8	30.0	2
Y	0.039	1.86	0.55	35.7	12.5	0.32	0.06	0.006	0.92	2.09	44.0	90.4	70.0	70
La	0.010	0.25	0.11	0.26	0.7	0.33	0.30	0.053	0.67	3.60	23.5	2.86	36.0	1710
Ce	0.016	0.50	0.15	0.35	1.52	0.32	0.27	0.044	0.74	3.46	34.7	2.64	53.3	1458.
Nd	0.025	1.11	0.22	0.53	4.26	0.29	0.21	0.025	1.20	3.22	57.1	2.20	88.3	1040.
Sc	5.0	23.0	10.0	20.0	20.0	16.0	0.04	0.04	12.0	10.0		10.0		56.
V	0.15	4.7	2.0	8.0	10.0	50.0	0.02	0.55	50.0	35.0				
Cr	1.90	15.0	10.0	20.0	30.0	5.0	0.15	0.56	10.0	6.0		180.0		380.
Co	9.0	11.0	15.0	3.0	45.0	90.0	0.08	0.42	30.0	15.0		16.0		42.
Ni	19.0	6.0	8.0	0.6	10.0	13.0	0.08	1.60	10.0	10.0				
Zn	10.0	10.0	10.0	10.0	6.8	16.0	0.37	0.075	23.0	7.8		8.5		27.

Distribution coefficients MAFREE.MEL - Mafic rocks

	Ol	Cpx	Opx	Gt	Hb	Bi	Pl	Mt	Il	Ap	Sp
La	0.0005	0.11	0.0005	0.0020	0.14	0.035	0.140	0.015	0.098	9.30	0.032
Ce	0.0008	0.15	0.0009	0.0033	0.20	0.034	0.120	0.016	0.110	9.60	0.033
Pr	0.0010	0.23	0.0014	0.0109	0.26	0.033	0.100	0.021	0.124	9.80	0.035
Nd	0.0013	0.31	0.0019	0.0184	0.33	0.032	0.081	0.023	0.140	10.00	0.038
Sm	0.0019	0.50	0.0028	0.0823	0.52	0.031	0.067	0.024	0.150	10.16	0.051
Eu	0.0019	0.51	0.0036	0.133	0.59	0.030	0.340	0.025	0.100	6.93	0.055
Gd	0.0019	0.61	0.0049	0.199	0.63	0.030	0.063	0.021	0.140	10.95	0.074
Tb	0.0019	0.645	0.0059	0.257	0.63	0.030	0.059	0.019	0.140	10.93	0.091
Dy	0.0020	0.68	0.0074	0.670	0.64	0.030	0.055	0.018	0.135	10.10	0.105
Ho	0.0020	0.665	0.0089	1.083	0.60	0.032	0.059	0.017	0.130	9.60	0.108
Er	0.0027	0.65	0.0155	2.05	0.55	0.034	0.063	0.017	0.141	8.40	0.110
Tm	0.0033	0.635	0.0221	3.03	0.52	0.038	0.065	0.018	0.155	7.40	0.108
Yb	0.0040	0.62	0.0286	4.00	0.49	0.042	0.067	0.018	0.170	6.45	0.105
Lu	0.0048	0.56	0.038	7.00	0.43	0.046	0.060	0.018	0.186	5.65	0.090

Distribution coefficients INTREE.MEL - Intermediate rocks

	Ol	Cpx	Opx	Gt	Hb	Bi	Pl	Ksp	Mt	Il	Ap	Z
La	0.005	0.16	0.06	0.26	0.44	0.180	0.212	0.053	0.247	1.85	10.0	0.28
Ce	0.008	0.27	0.08	0.35	0.90	0.180	0.150	0.044	0.291	1.78	12.0	0.27
Pr	0.011	0.43	0.10	0.44	1.85	0.170	0.127	0.035	0.338	1.73	13.8	0.265
Nd	0.013	0.60	0.11	0.53	2.80	0.160	0.108	0.025	0.396	1.67	16.0	0.26
Sm	0.019	0.90	0.14	2.66	3.99	0.145	0.081	0.018	0.423	1.49	20.0	0.87
Eu	0.019	0.86	0.09	1.50	3.44	0.135	0.975	1.13	0.270	0.33	11.4	0.18
Gd	0.019	1.02	0.17	10.5	5.48	0.155	0.058	0.011	0.405	1.35	20.0	4.70
Tb	0.019	1.04	0.20	19.6	5.84	0.155	0.053	0.008	0.397	1.30	18.0	10.8
Dy	0.020	1.06	0.23	28.6	6.20	0.160	0.048	0.006	0.392	1.21	16.0	25.2
Ho	0.020	1.03	0.28	35.7	6.07	0.175	0.042	0.006	0.341	1.11	13.8	45.0
Er	0.028	1.00	0.33	42.8.	5.94	0.190	0.036	0.006	0.299	1.04	12.0	81.5
Tm	0.034	0.95	0.39	41.4	5.41	0.220	0.031	0.006	0.261	0.97	9.8	120.0
Yb	0.041	0.89	0.44	39.9	4.89	0.240	0.027	0.006	0.229	0.90	8.0	178.0
Lu	0.049	0.87	0.47	29.6	4.53	0.250	0.025	0.006	0.178	0.66	6.0	260.0

Distribution coefficients FELREE.MEL - Felsic rocks

	Ol	Cpx	Opx	Gt	Hb	Bi	Pl	Ksp	Mt	Il	Ap	Z	Sph	All
La	0.010	0.25	0.11	0.26	0.70	0.330	0.300	0.053	0.670	3.60	23.5	2.86	36.0	1710.
Ce	0.016	0.50	0.15	0.35	1.52	0.320	0.270	0.044	0.740	3.46	34.7	2.64	53.3	1458.
Pr	0.020	0.80	0.19	0.44	2.89	0.310	0.240	0.035	0.940	3.34	45.9	2.42	74.0	1249.
Nd	0.025	1.11	0.22	0.53	4.26	0.290	0.210	0.025	1.200	3.22	57.1	2.20	88.3	1040.
Sm	0.037	1.67	0.27	2.66	7.77	0.260	0.130	0.018	1.400	2.83	62.8	3.14	102.0	538.
Eu	0.037	1.56	0.17	1.50	5.14	0.240	2.520	1.87	0.480	0.55	30.4	3.14	101.0	95.
Gd	0.037	1.85	0.34	10.5	10.00	0.280	0.097	0.011	1.300	2.57	56.3	12.0	102.0	300.
Tb	0.037	1.89	0.40	19.6	11.50	0.280	0.080	0.008	1.240	2.47	53.5	28.9	91.0	170.
Dy	0.039	1.93	0.46	28.6	13.00	0.290	0.064	0.006	1.120	2.28	50.7	45.7	80.6	86.
Ho	0.039	1.86	0.55	35.7	12.50	0.320	0.060	0.006	0.920	2.09	44.0	90.4	70.0	70
Er	0.053	1.80	0.65	42.8	12.00	0.350	0.055	0.006	0.750	1.93	37.2	135.0	58.7	53.
Tm	0.064	1.69	0.76	41.4	10.20	0.400	0.052	0.006	0.610	1.78	30.6	200.0	48.0	36.
Yb	0.078	1.58	0.86	39.9	8.38	0.440	0.049	0.006	0.590	1.64	23.9	270.0	37.4	20
Lu	0.094	1.54	0.90	29.6	5.50	0.460	0.046	0.006	0.590	1.14	20.2	323.0	26.9	20.

APPENDIX D. GRAPHICS OVERLAY FILES

Graphics overlay files are used to add extra information , such as text and field boundaries, to XY and triangular plots. In particular, field boundaries used in various rock classifications can easily be superimposed on the appropriate plot.

The format of a typical file is as follows:

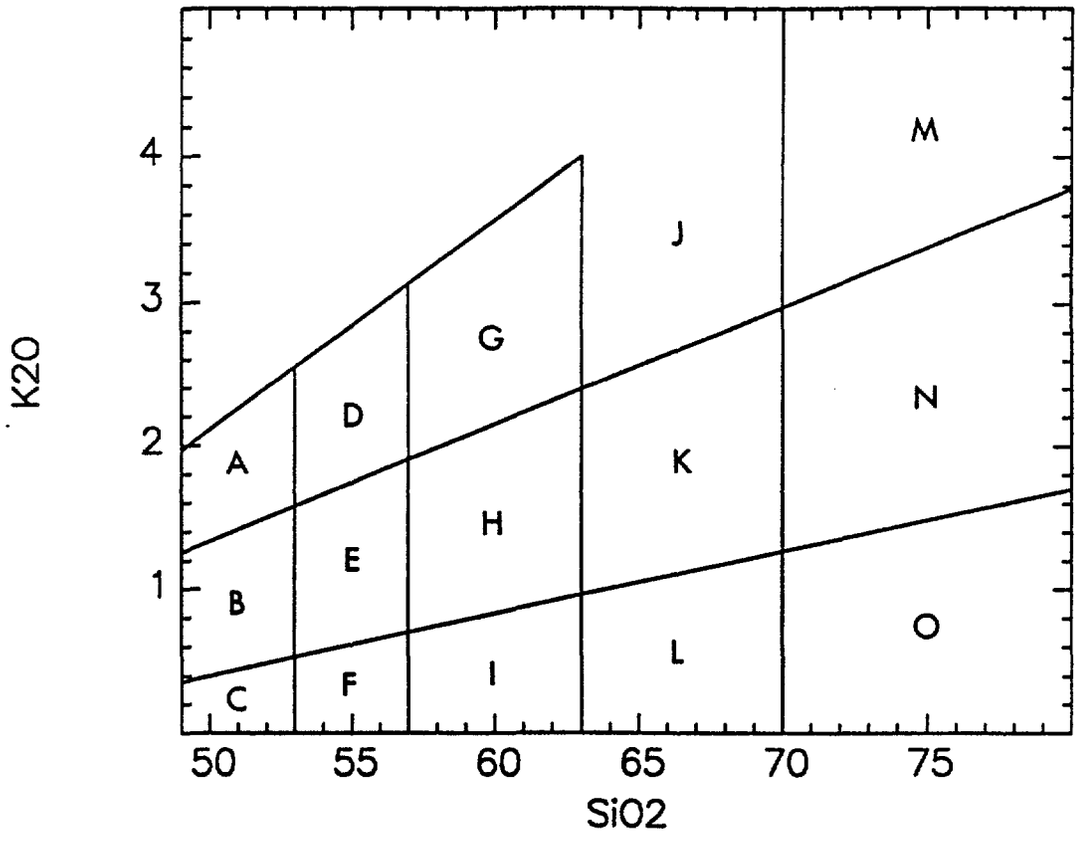
```
Graphics overlay file - tstgda.grf
*Example file - space for comments
Font        11
Pen         4
Textsize
1.0
Text
Granite field
68.0,0.2
Pen         1
Linetype    2
Line        3
68.0,0.2
70.0,0.5
79.0,0.9
Pen         2
Linetype    2
Line        2
68.0,0.2
99.0,0.4
Pen         3
Symbolsize
0.8
Symbol      6
70.0, 0.5
```

The first line, which specifies the file type, is mandatory, and any lines beginning with a * are used for explanatory comments. Text can be displayed by specifying font, pen colour, and textsize, followed by the text itself and the XY co-ordinates of the beginning of the text. Symbols require pen colour, symbolsize and symbol number, followed by the XY co-ordinates. Lines require pen colour, linetype number, and the number of co-ordinate pairs (X, Y) needed to define the line, followed by the same number of co-ordinates. For straight lines, only the beginning, and end co-ordinates, and, if appropriate, the co-ordinates of each intermediate change of orientation (kink) need be given. For example, a V-shaped line would require three co-ordinate pairs. Curved lines require a relatively large number of closely spaced co-ordinates. Any number of intersecting or parallel lines may be specified. Note that it is only necessary to re-

define the font, symbol, linetype, pen, textsize, and symbolsize if these need to be changed. Font, pen, symbol, and linetype numbers are given in the 11-15 character field on the same line, whereas decimal values (symbolsize and textsize) must be on the following line. Each XY co-ordinate is separated by a comma. Only the X (left) and Y (upper) co-ordinates should be given for triangular plots. If the axes limits selected for XY plots are less than those covered by the overlay file, lines will be truncated on the screen, but not necessarily on the paper plots (correction fluid may have to be used!).

The following pages list the presently available graphics overlay files, which include some of those commonly used for rock classification. All have a name with the extension .GRF. In most cases, text has not been included in the files, as this would inevitably tend to be superimposed on the plot points.

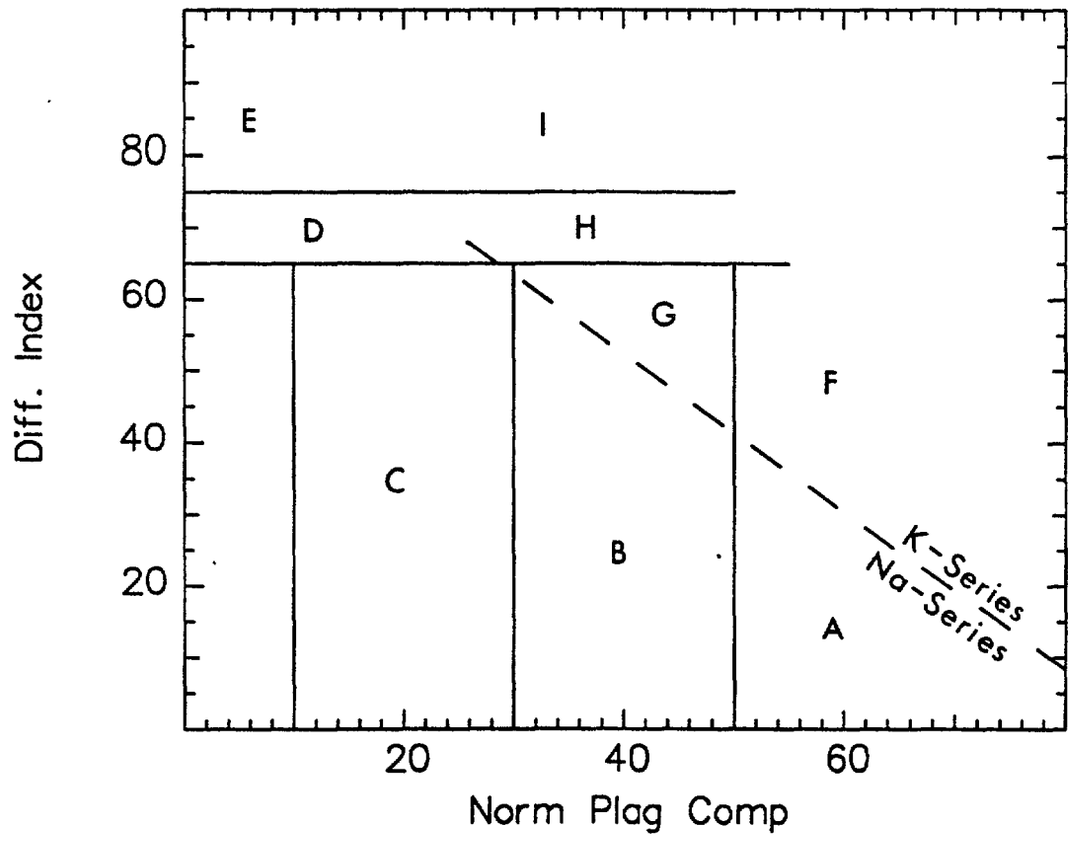
```
Graphics overlay file - KSIL.GRF
*K2O-SiO2 classification of volcanic rocks:
*Peccerillo & Taylor (1976),
*modified after Gill (1981)
Pen             1
Linetype        1
Line            2
49.0,1.97
63.0,4.00
Line            2
49.0,1.25
80.0,3.79
Line            2
49.0,0.36
80.0,1.70
Line            2
53.0,0.00
53.0,2.55
Line            2
57.0,0.00
57.0,3.13
Line            2
63.0,0.00
63.0,4.00
Line            2
70.0,0.00
70.0,5.00
```



KSIL.GRF (Peccerillo & Taylor, 1976; Gill, 1981)

A. High-K basalt
B. Basalt
C. Low-K tholeiite
D. High-K basaltic andesite
E. Basaltic andesite
F. Low-K basaltic andesite
G. High-K andesite
H. Andesite
I. Low-K andesite
J. High-K dacite
K. Dacite
L. Low-K dacite
M. High-K rhyolite
N. Rhyolite
O. Low-K rhyolite

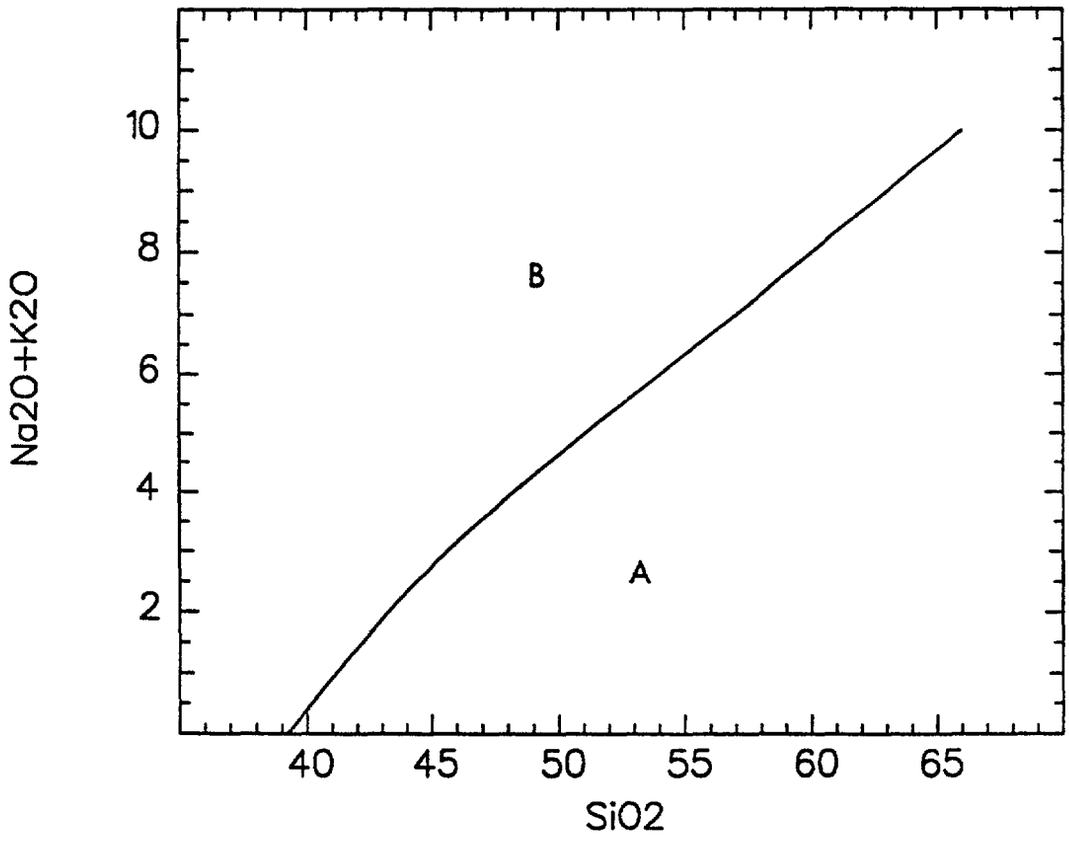
```
Graphics overlay file - PLAGDI.GRF
*%An-Differentiation Index classification of potassic
*and sodic alkaline volcanic rocks:
*Coombs & Wilkinson (1969)
Pen         1
Linetype    1
Line        2
0.0,65.0
55.0,65.0
Line        2
0.0,75.0
50.0,75.0
Line        2
50.0,0.0
50.0,65.0
Line        2
30.0,0.0
30.0,65.0
Line        2
10.0,0.0
10.0,65.0
Linetype    2
Line        2
80.0,8.4
24.0,70.0
```



PLAGDI.GRF (Coombs & Wilkinson, 1969)

A. Basalt
B. Hawaiite
C. Mugearite
D. Benmoreite
E. Trachyte
F. K-basalt
G. Trachyandesite
H. Tristanite
J. K-trachyte

```
Graphics overlay file - ALKSIL.GRF
*Na2O+K2O - SiO2 classification of alkaline
*and sub-alkaline volcanic rocks:
*Irvine & Baragar (1971)
Pen         1
Linetype    1
Line        15
39.25,0.0
40.00,0.4
40.75,0.8
41.55,1.2
42.40,1.6
43.25,2.0
44.15,2.4
45.10,2.8
46.10,3.2
47.15,3.6
48.20,4.0
49.30,4.4
50.45,4.8
51.60,5.2
66.00,10.0
```

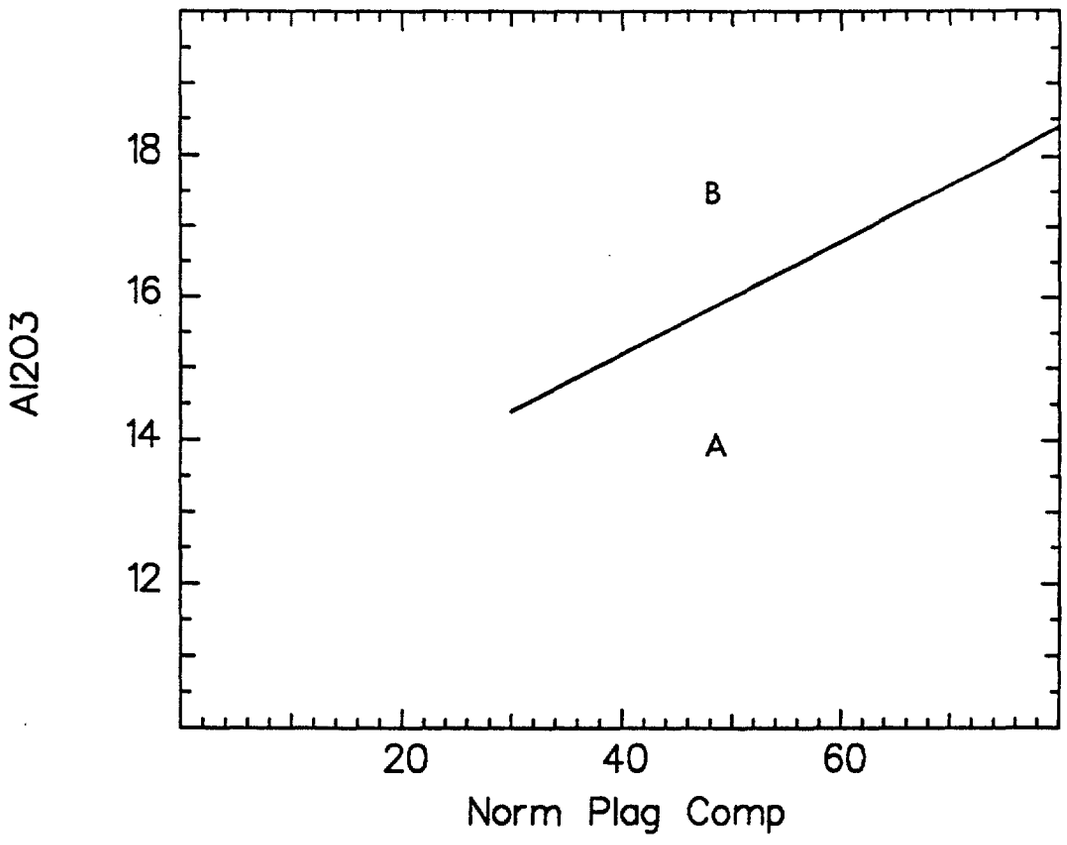


ALKSIL.GRF (Irvine & Baragar 1971)

A. Subalkaline volcanics

B. Alkaline volcanics

```
 Graphics overlay file - PLAGAL.GRF
*Al2O3-%An classification of tholeiitic and
*calc-alkaline volcanic rocks:
*Irvine & Baragar (1971)
Pen         1
Linetype    1
Line        2
80.0,18.4
30.0,14.4
```

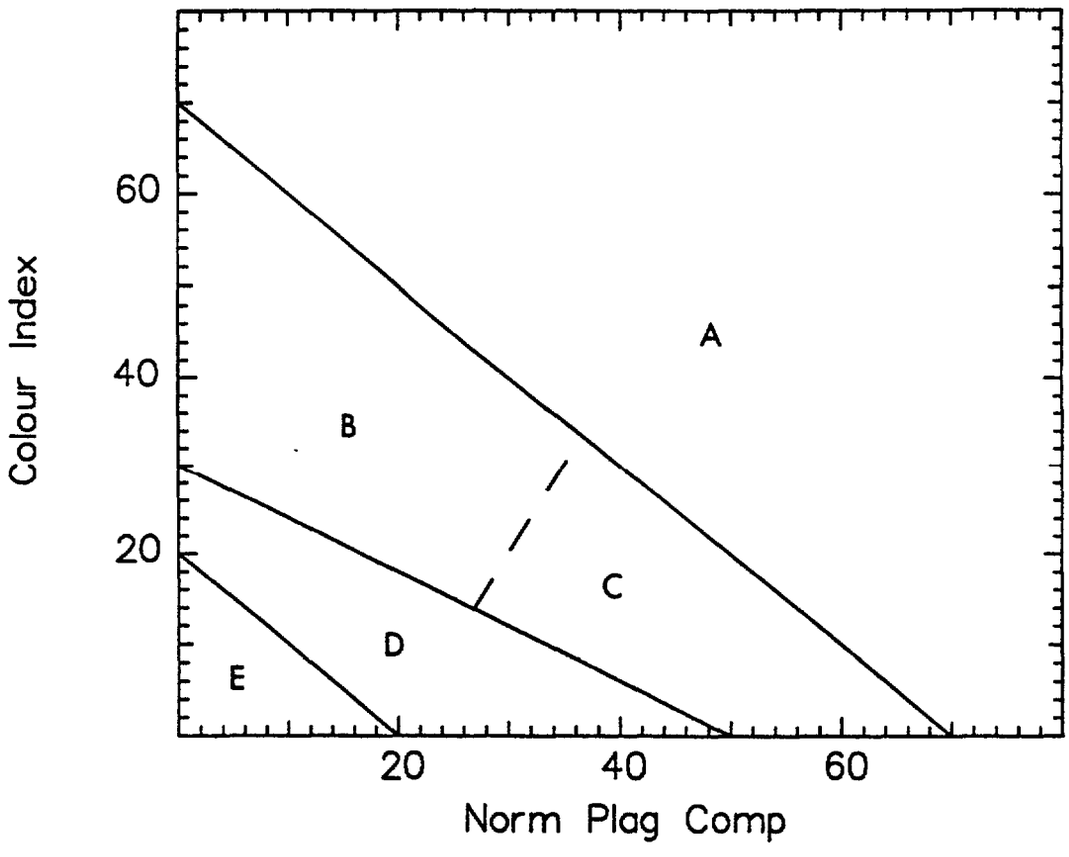


PLAGAL.GRF (Irvine & Baragar, 1971)

A. Tholeiitic volcanics

B. Calc-alkaline volcanics

```
Graphics overlay file - PLAGCI.GRF
*%An-Colour Index classification of
*sub-alkaline volcanic rocks:
*Irvine & Baragar (1971)
Pen         1
Linetype    1
Line        2
70.0,0.0
0.0,70.0
Line        2
50.0,0.0
0.0,30.0
Line        2
20.0,0.0
0.0,20.0
Linetype    2
Line        2
26.9,13.8
36.6,33.4
```



PLAGCI.GRF (Irvine & Baragar, 1971)

A. Basalt

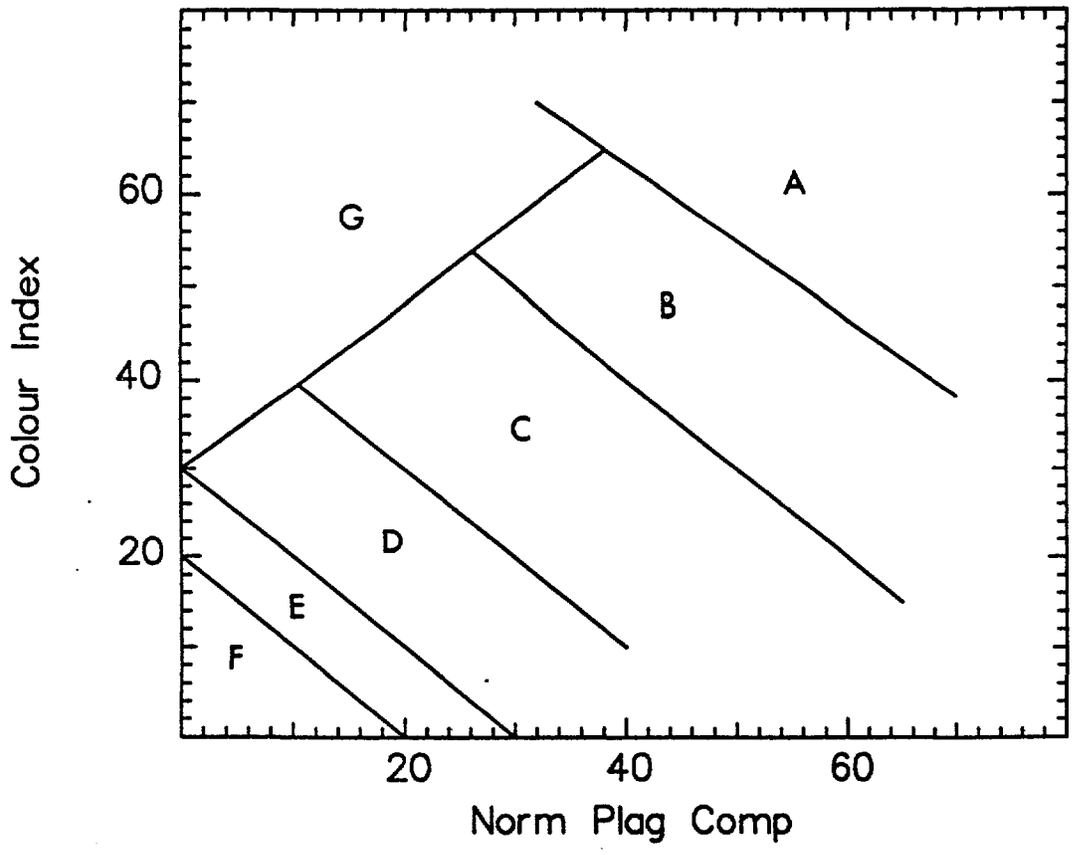
B. Tholeiitic andesite

C. Andesite

D. Dacite

E. Rhyolite

```
Graphics overlay file - NAPLCI.GRF
*100An/(An+Ab+1.85Ne)-Colour Index classification
*of low-K alkaline volcanic rocks:
*Irvine & Baragar (1971)
Pen         1
Linetype    1
Line        2
70.0,38.3
32.0,70.0
Line        2
65.0,15.0
26.15,53.85
Line        2
40.0,10.0
10.5,39.5
Line        2
30.0,0.0
0.0,30.0
Line        2
20.0,0.0
0.0,20.0
Line        2
0.0,30.0
38.2,64.9
```



NAPLCI.GRF (Irvine & Baragar, 1971)

A. Picrite-basalt, ankaramite

B. Alkali basalt

C. Hawaiite

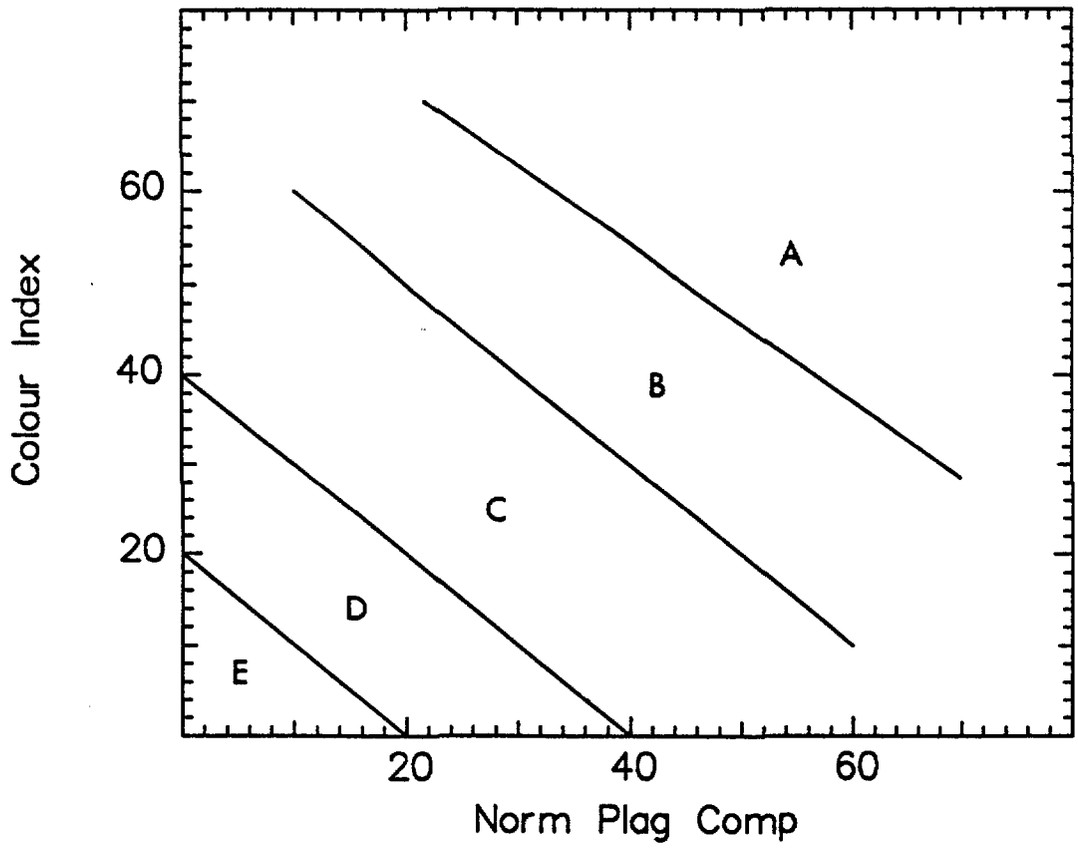
D. Mugearite

E. Benmorite

F. Trachyte

G. Nephelinite

```
   Graphics overlay file - KPLCI.GRF
*100An/(An+Ab+1.85Ne)-Colour Index classification
*of high-K alkaline volcanic rocks:
*Irvine & Baragar (1971)
Pen         1
Linetype    1
Line        2
70.0,28.6
21.67,70.0
Line        2
60.0,10.0
10.0,60.0
Line        2
40.0,0.0
0.0,40.0
Line        2
20.0,0.0
0.0,20.0
```



KPLCI . GRF (Irvine & Baragar, 1971)

A. Picrite-basalt, ankaramite

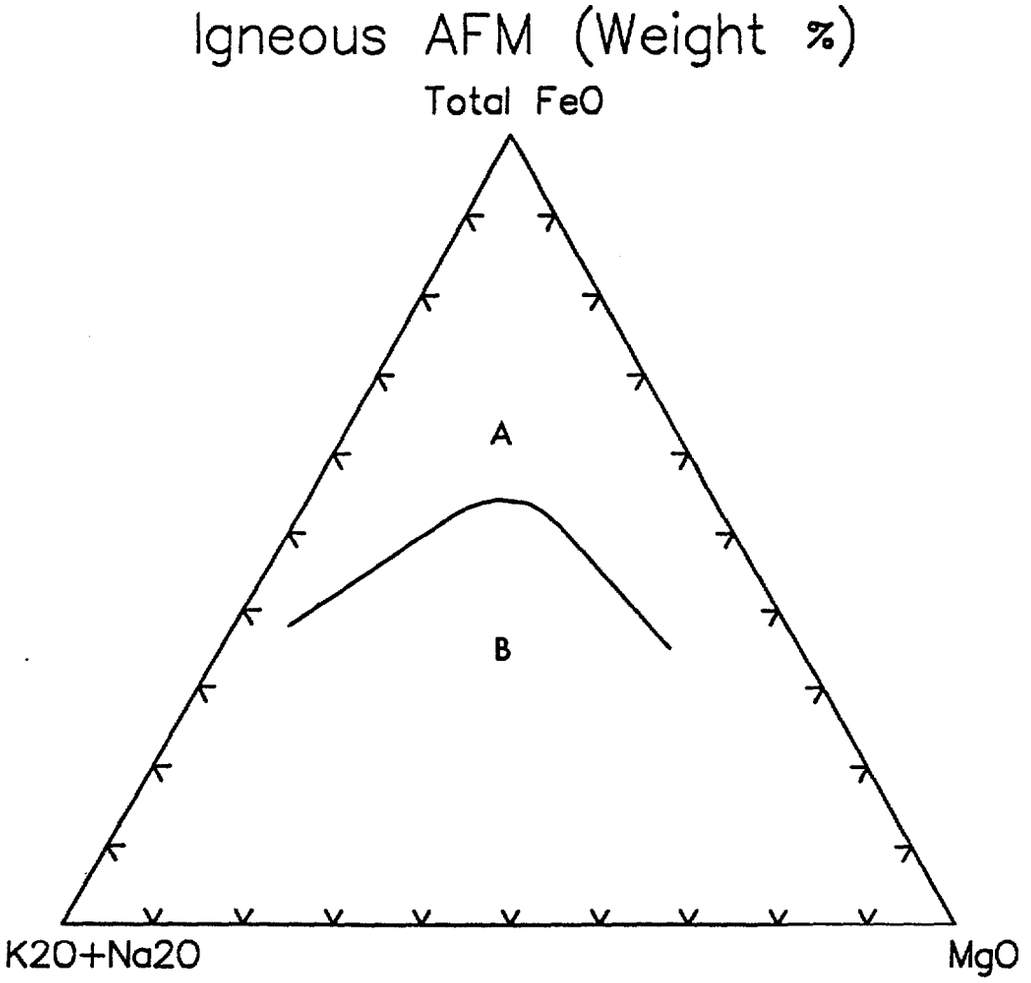
B. Alkali basalt

C. Trachybasalt

D. Tristanite

E. Trachyte

```
Graphics overlay file - AFM.GRF
*Na2O+K2O - Total FeO - MgO classification of
*tholeiitic and other volcanic rocks:
*Irvine & Baragar (1971)
Pen         1
Linetype    1
Line        17
55.9,38.0
30.0,52.5
29.0,53.0
28.0,53.4
27.0,53.8
26.0,54.1
25.0,54.3
24.0,54.4
23.0,54.3
22.0,54.2
21.1,53.9
20.5,53.5
20.0,53.0
19.6,52.4
19.3,51.7
19.0,51.0
14.6,35.0
```

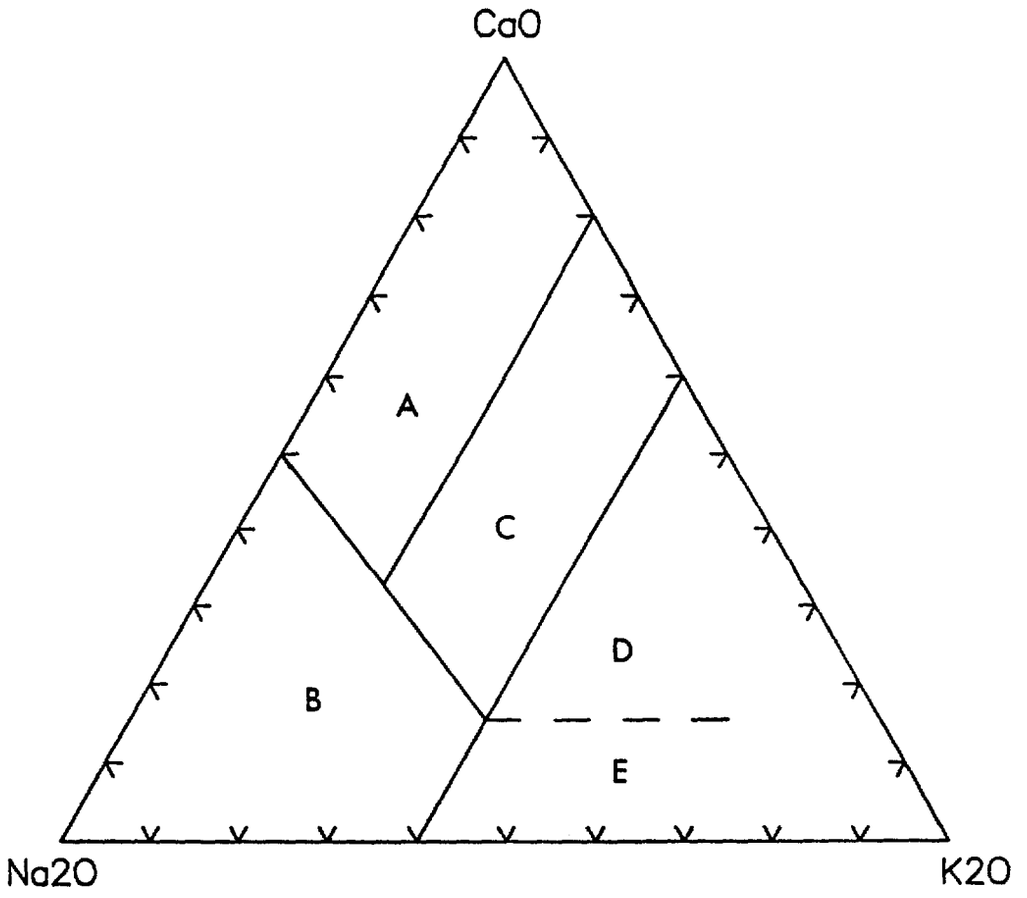


AFM.GRF (Irvine & Baragar, 1971)

A. Tholeiitic volcanics

B. Alkaline and calc-alkaline volcanics

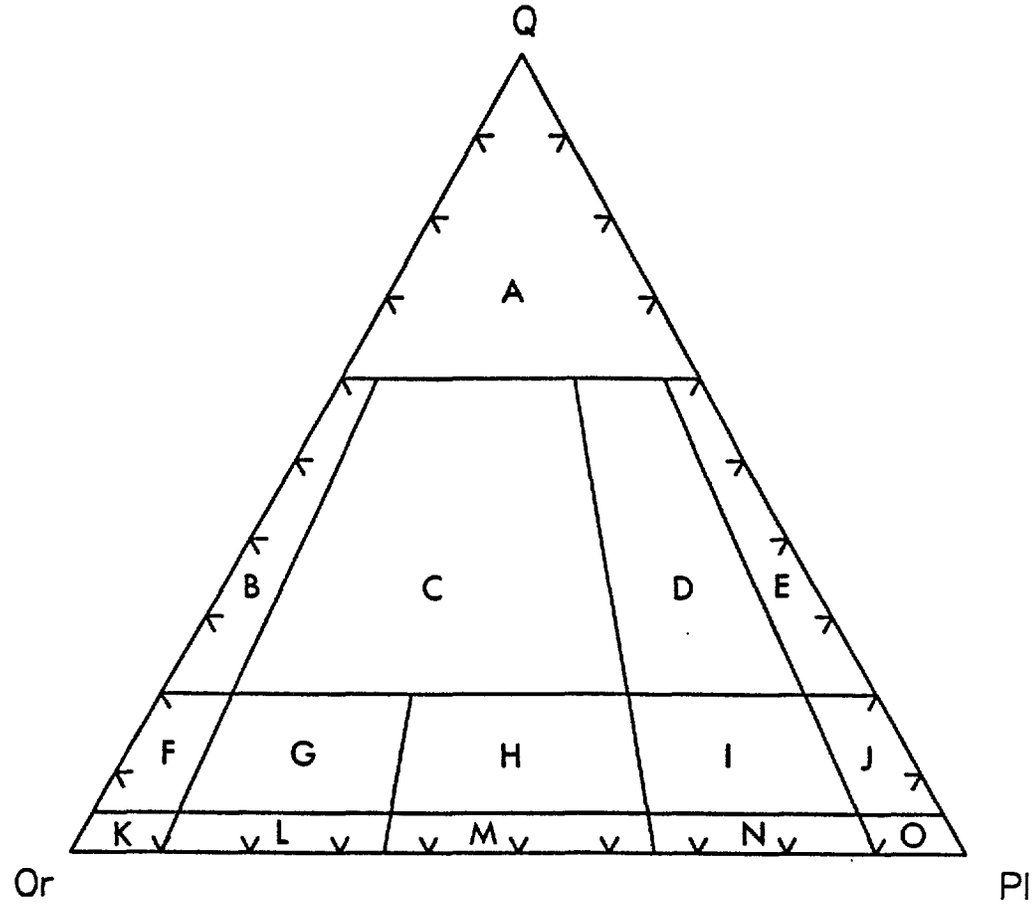
```
Graphics overlay file - CANAK.GRF
*CaO-Na2O-K2O classification of
*felsic igneous rocks:
*A. J. R. White (pers. comm., 1988)
Pen         1
Linetype    1
Line        2
50.0,50.0
44.5,15.5
Line        2
0.0,60.0
60.0,0.0
Line        2
0.0,80.0
47.3,32.7
Linetype    2
Line        2
44.5,15.5
17.0,15.5
```



CANAK.GRF (A.J.R. White, personal communication, 1988)

Plutonic Rocks	Volcanic Rocks
A. Tonalite	A. Dacite
B. Trondhjemite	B. Keratophyre
C. Granodiorite	C. Dacite
D. Adamellite	D. Rhyolite
E. Granite	E. Rhyolite

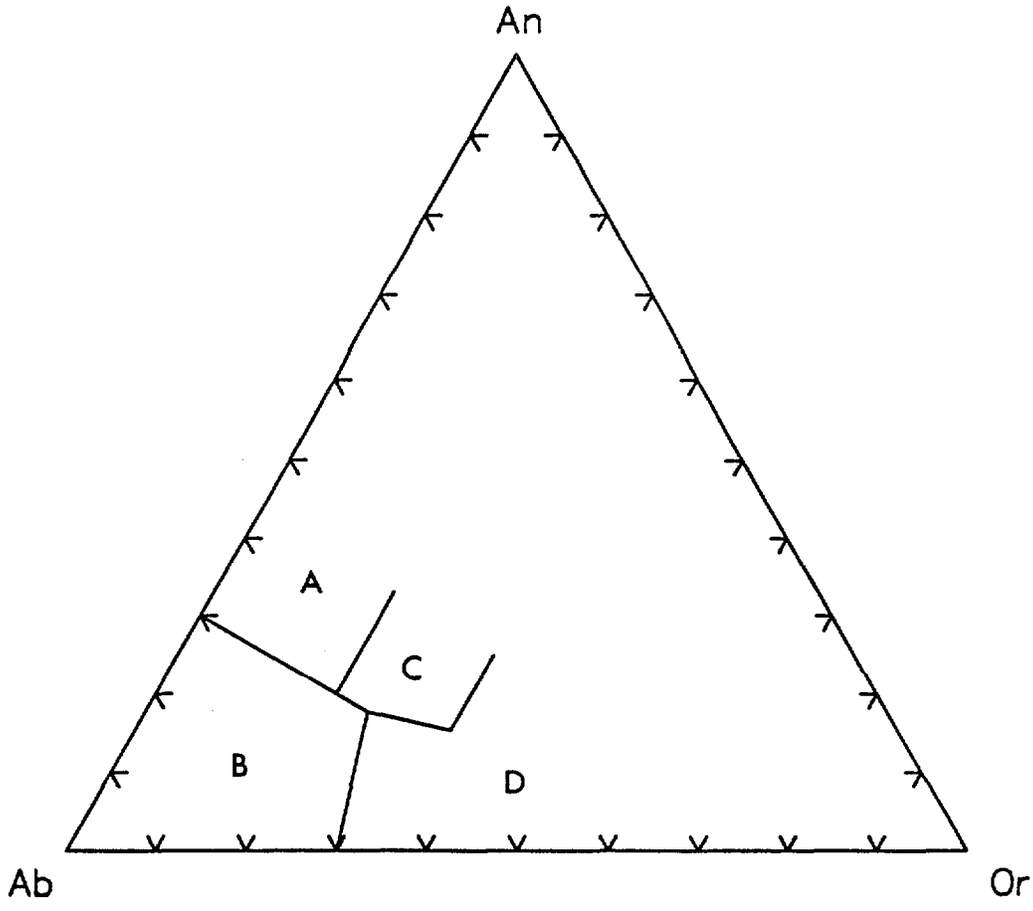
```
Graphics overlay file - STRECK.GRF
*Quartz-Alkali Feldspar-Plagioclase classification
*of plutonic and volcanic rocks (strictly only
*applicable to modal compositions):
*Streckeisen (1973,1976,1979)
Pen         1
Linetype    1
Line        2
40.0,60.0
0.0,60.0
Line        2
80.0,20.0
0.0,20.0
Line        2
95.0,5.0
0.0,5.0
Line        2
36.0,60.0
90.0,0.0
Line        2
4.0,60.0
10.0,0.0
Line        2
14.0,60.0
35.0,0.0
Line        2
52.0,20.0
65.0,0.0
```



STRECK.GRF (STRECKEISEN, 1973, 1976, 1979)

Plutonic Rocks	Volcanic Rocks
A. Quartz-rich granitoids	A. Quartz-rich rhyolites
B, Alkali-feldspar granite	B. Alkali(-feldspar) rhyolite
C. Granite	C. Rhyolite
D. Granodiorite	D. Dacite
E. Tonalite	E. Dacite
F. Alkali-feldspar quartz syenite	F. Quartz-alkali(-feldspar) trachyte
G. Quartz syenite	G. Quartz trachyte
H. Quartz monzonite	H. Quartz latite
I. Quartz monzodiorite/quartz monzogabbro	I. Andesite/basalt
J. Quartz diorite/quartz gabbro/quartz anorthosite	J. Andesite/basalt
K. Alkali-feldspar syenite	K. Alkali(-feldspar) trachyte
L. Syenite	L. Trachyte
M. Monzonite	M. Latite
N. Monzodiorite/monzogabbro	N. Andesite/basalt
O. Diorite/gabbro/anorthosite	O. Andesite/basalt

```
Graphics overlay file - BARKER.GRF
*Normative Ab-Or-An classification
*of granitic rocks:
*Barker (1979)
Pen        1
Linetype   1
Line       3
70.0,30.0
57.7,17.7
49.6,15.4
Line       2
49.6,15.4
40.0,25.0
Line       2
60.0,20.0
47.0,33.0
Line       2
57.7,17.7
70.0,0.0
```



BARKER . GRF (Barker, 1979)

A. Tonalite

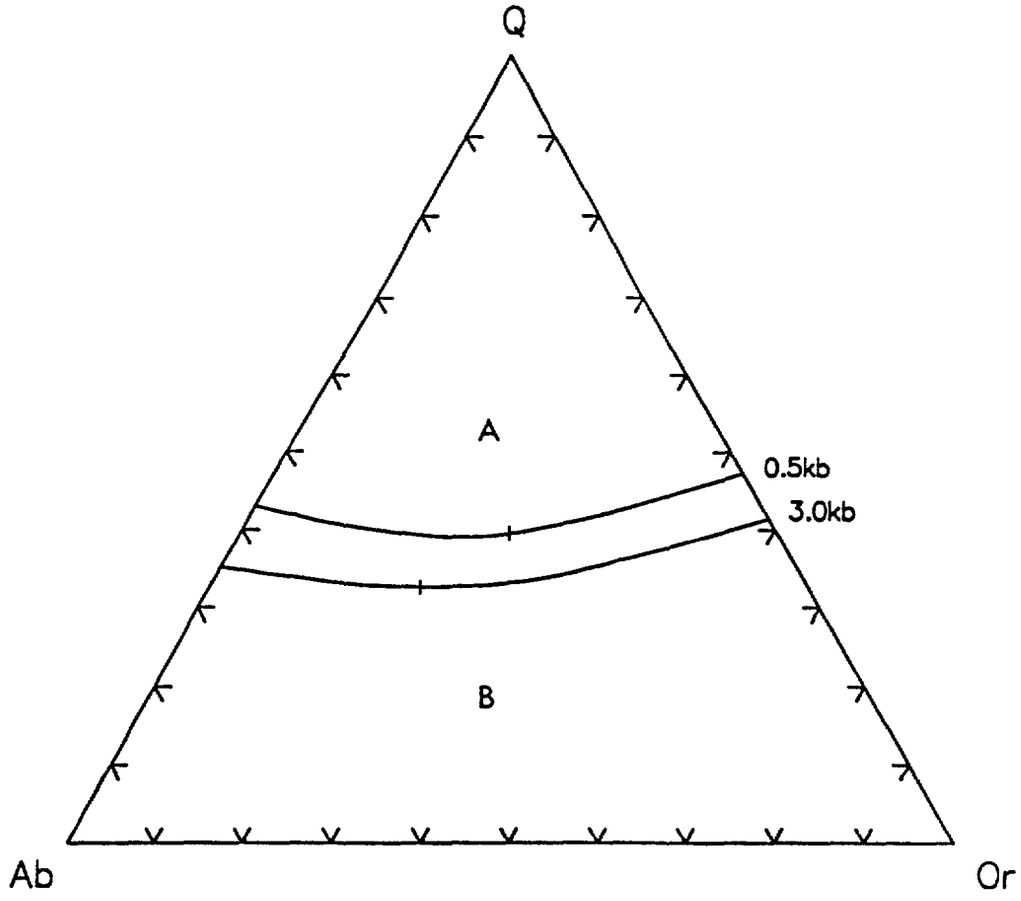
B. Trondhjemite

C. Granodiorite

D. Granite

```
Graphics overlay file - QABOR.GRF
*Normative Q-Ab-Or diagram showing quartz-feldspar
*field boundaries at 0.5 and 3.0kbars PH2O and
*positions of quaternary isobaric minima:
*Tuttle & Bowen (1958)
Pen       1
Linetype  1
Line      23
57.0,43.0
55.0,42.4
53.0,41.8
51.0,41.2
49.0,40.7
47.0,40.3
45.0,40.0
43.0,39.7
41.0,39.4
39.0,39.2
37.0,39.1
35.0,39.1
33.0,39.2
31.0,39.4
29.0,39.7
27.0,40.1
25.0,40.5
23.0,40.9
21.0,41.3
19.0,41.8
17.0,42.3
15.0,42.8
0.0,47.2
Line      2
29.9,40.3
30.7,38.7
Line      27
64.8,35.2
60.0,34.3
58.0,34.0
56.0,33.7
54.0,33.4
52.0,33.1
50.0,32.9
48.0,32.8
46.0,32.7
44.0,32.6
42.0,32.6
40.0,32.7
38.0,32.8
36.0,32.9
34.0,33.1
32.0,33.3
30.0,33.6
28.0,34.0
26.0,34.4
24.0,34.9
22.0,35.4
20.0,35.9
18.0,36.4
16.0,36.9
14.0,37.4
12.0,38.0
0.0,41.4
Line      2
43.4,33.4
```

```
44.2,31.8
Font        5
Pen         1
Textsize
0.7
Text
0.5kb
-1.5,46.0
Text
3.0kb
-1.5,40.4
```

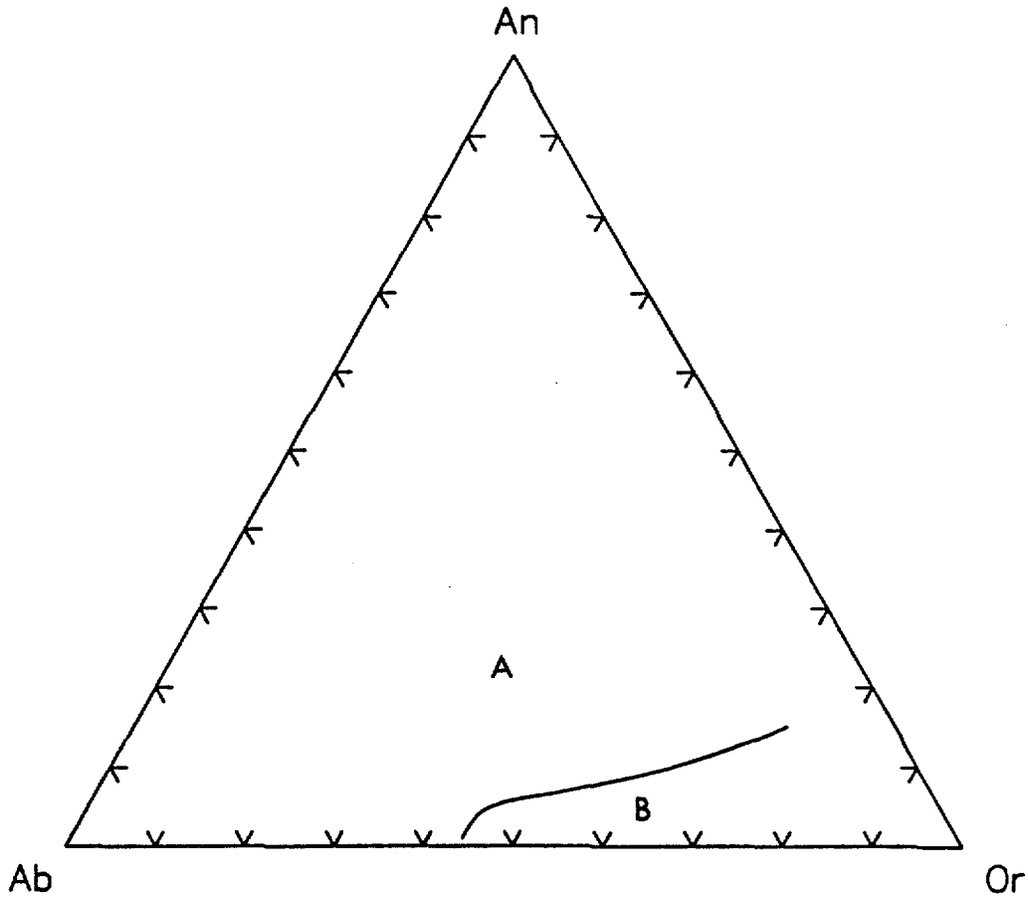


QABOR . GRF (Tuttle & Bowen, 1958)

A. Quartz

B. Feldspar

```
Graphics overlay file - ABORAN.GRF
*Normative Ab-Or-An diagram showing plagioclase-
*alkali-feldspar field boundary at 1000bars PH2O,
*projected onto the Ab-Or-An face of the tetrahedron
*in the quartz-saturated ternary feldspar system:
*James & Hamilton (1969)
Pen         1
Linetype    1
Line        25
55.1,1.0
54.1,2.0
53.0,3.0
51.8,4.0
51.0,4.5
50.0,4.9
48.0,5.6
46.0,6.0
44.0,6.3
42.0,6.7
40.0,7.1
38.0,7.5
36.0,8.0
34.0,8.4
32.0,8.8
30.0,9.3
28.0,9.8
26.0,10.4
24.0,11.0
22.0,11.6
20.0,12.2
18.0,12.9
16.0,13.6
14.0,14.3
12.0,15.1
```

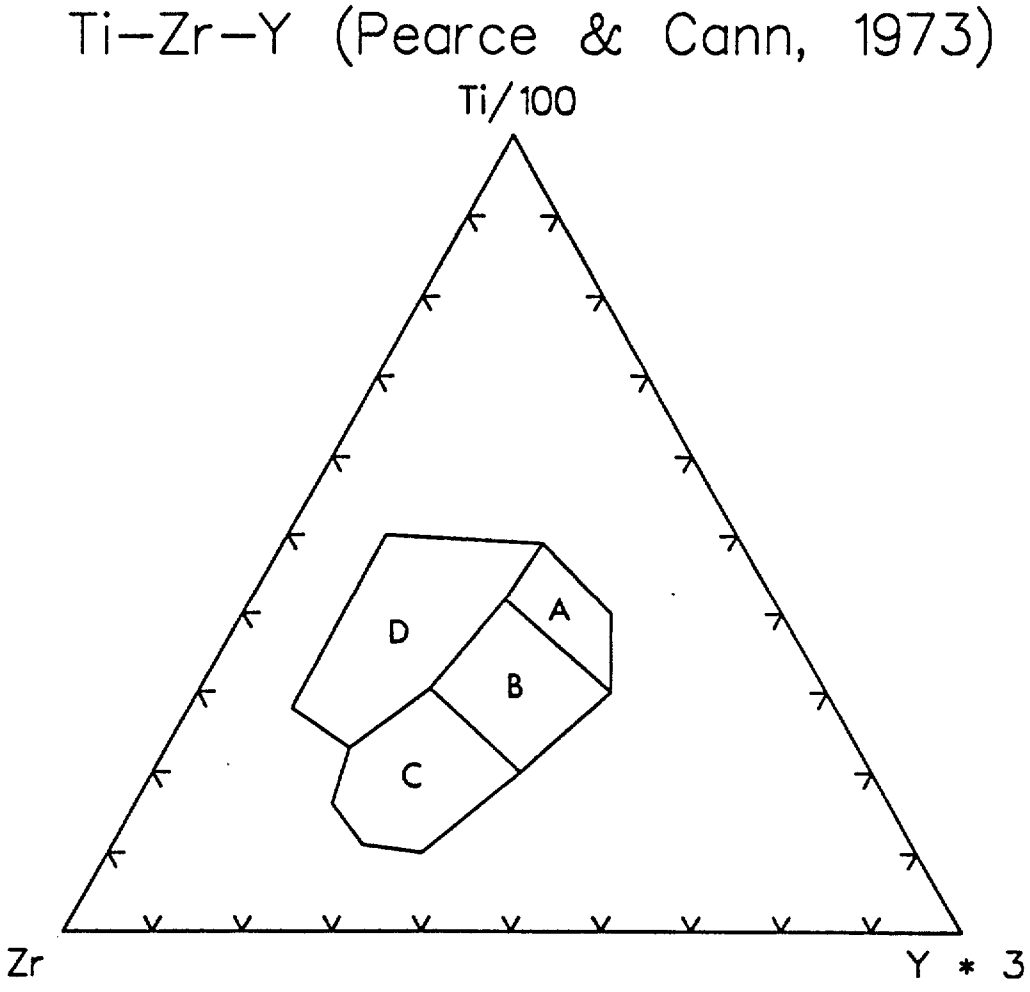


ABORAN . GRF (James & Hamilton, 1969)

A. Plagioclase

B. Alkali-feldspar

```
Graphics overlay file - TIZRY.GRF
*Ti/100-Zr-3Y classification of basalts:
*Pearce & Cann (1973)
Pen         1
Linetype    1
Line        11
39.0,50.0
22.0,49.0
19.0,40.0
24.0,30.0
39.0,20.0
55.0,10.0
61.0,11.0
62.0,16.0
56.5,23.0
60.5,28.0
39.0,50.0
Line        4
22.0,49.0
29.8,41.8
43.8,30.5
56.5,23.0
Line        2
29.8,41.8
24.0,30.0
Line        2
43.8,30.5
39.0,20.0
```



TIZRY . GRF (Pearce & Cann, 1973)

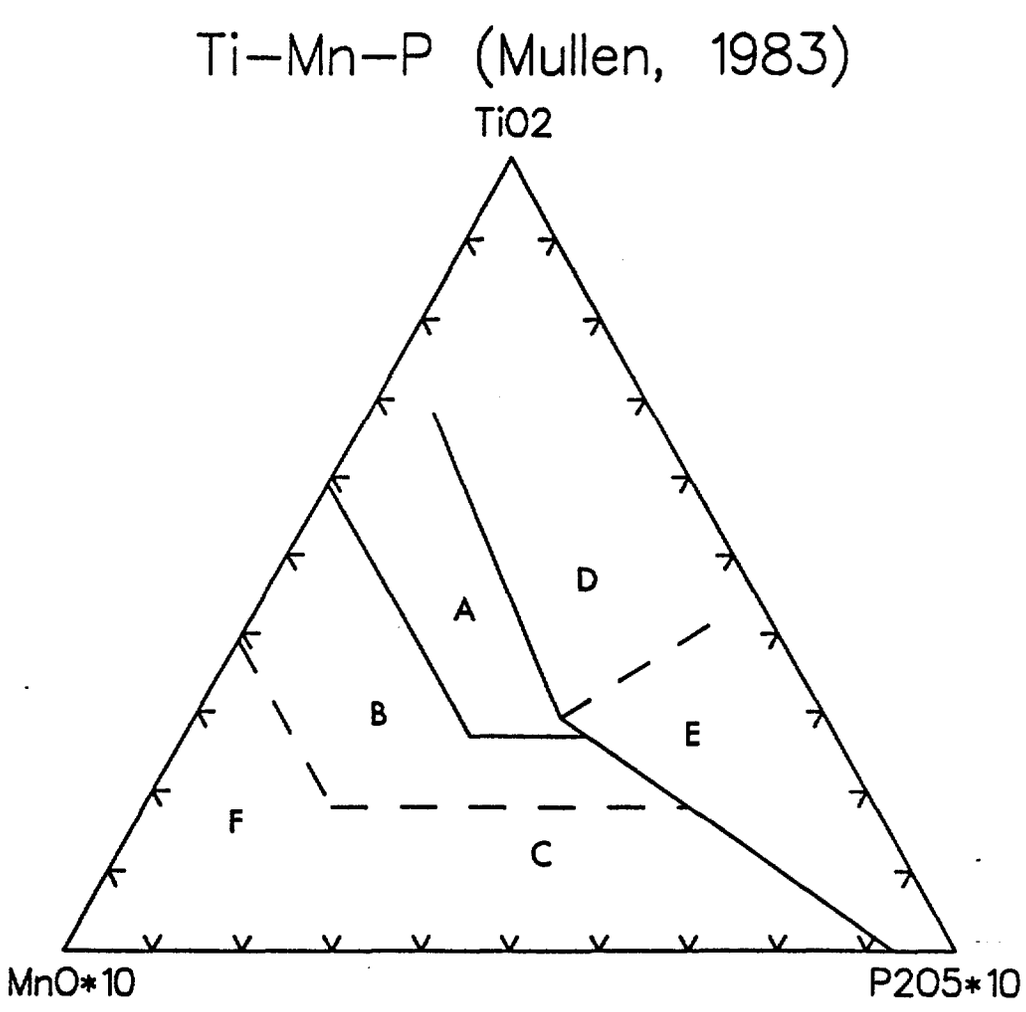
A,B. Low-K (island arc) tholeiites

B. Ocean-floor basalts

B,C. Calc-alkali basalts (island arc)

D. Within-plate basalts (ocean island and continental basalts)

```
Graphics overlay file - TIMNP.GRF
*TiO2-10MnO-10P2O5 classification of oceanic basalts:
*Mullen (1983)
Pen         1
Linetype    1
Line        3
24.6,68.2
29.7,29.3
7.0,0.0
Line        3
41.0,59.0
41.0,27.0
28.0,27.0
Linetype    2
Line        3
61.0,39.0
61.0,18.0
21.0,18.0
Line        2
29.7,29.3
5.5,42.0
```



TIMNP.GRF (Mullen, 1983)

A. Mid-ocean ridge basalt (MORB)

B. Island arc tholeiite

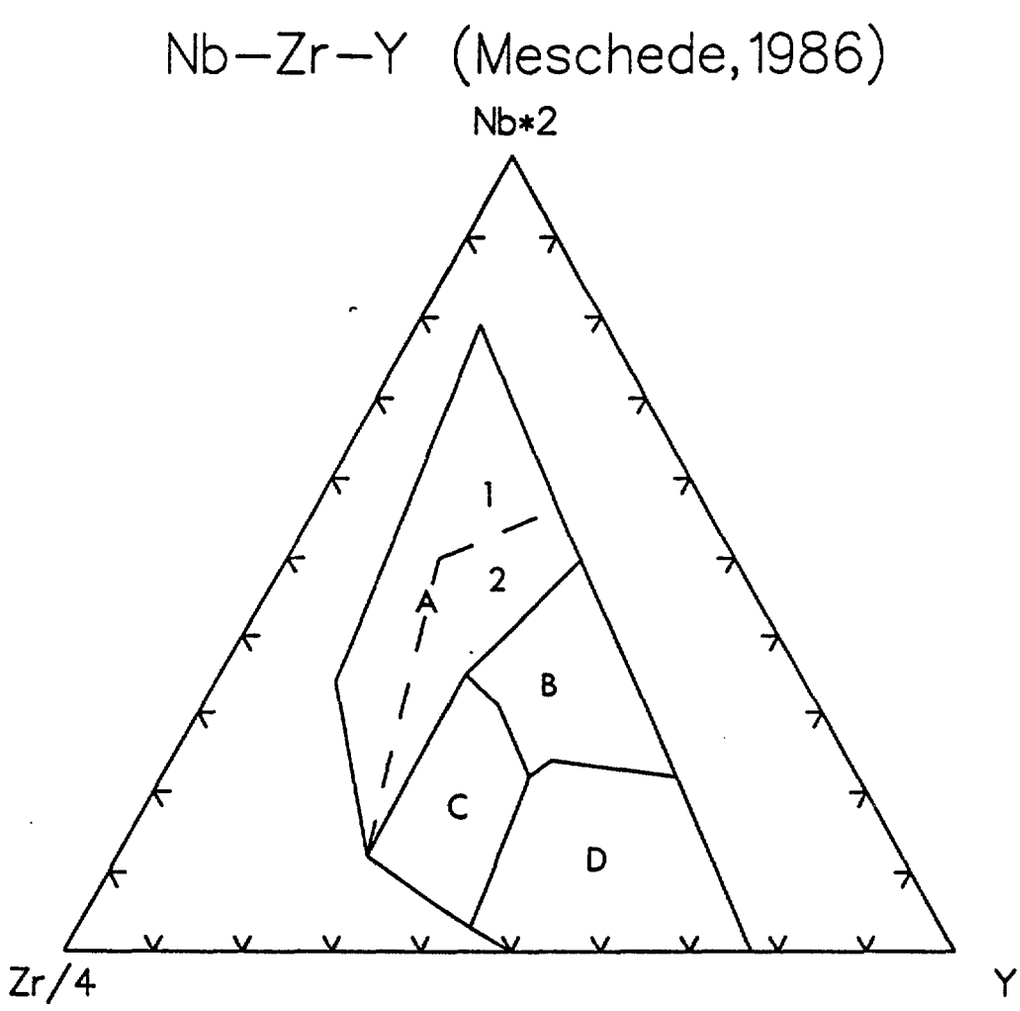
C. Island arc calc-alkaline basalt

D. Ocean island tholeiite

E. Ocean island alkali basalt

F. Boninite

```
Graphics overlay file - NBZRY.GRF
*2Nb-Zr/4-Y classification of basalts:
*Meschede (1986)
Pen         1
Linetype    1
Line        6
50.0,0.0
53.0,3.0
60.0,12.0
52.5,34.0
14.0,79.0
23.0,0.0
Line        3
60.0,12.0
37.5,35.0
17.3,49.6
Line        4
53.0,3.0
37.0,22.0
33.5,24.0
20.5,22.0
Line        3
37.0,22.0
36.0,31.0
37.5,35.0
Linetype    2
Line        3
60.0,12.0
33.0,50.0
16.5,56.5
```



NBZRY . GRF (Meschede, 1986)

A1,2. Within-plate alkali basalts

A2,C. Within-plate tholeiites

B. P-type MORB

D. N-type MORB

C,D. Volcanic arc basalts