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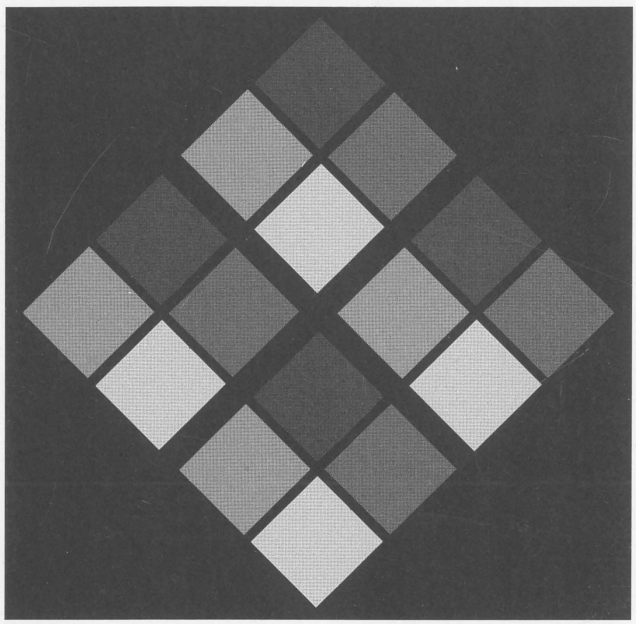
# MINERAL DATA ANALYSIS SYSTEM (MDA) REFERENCE MANUAL

## Record 1992/3





by AL Jaques, L Simons and JW Sheraton

Bureau of Mineral Resources, Geology and Geophysics

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MINERALS AND LAND USE PROGRAM

DEPARTMENT OF PRIMARY INDUSTRIES AND ENERGY

Minister: The Hon. Alan Griffiths

Secretary: G. L. Miller

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Executive Director: R.W.R. Rutland AO



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# NOTICE

While every effort has been made to ensure that the software is as error-free as possible, BMR cannot undertake to provide any formal software support to purchasers of the system if problems do arise. Nevertheless, we will attempt to assist users who encounter difficulties, and would appreciate being informed of any bugs which may become apparent. Please refer enquiries about the software to

Dr John Sheraton or Dr Doone Wyborn

Minerals and Land Use Program

Bureau of Mineral Resources

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CANBERRA ACT 2601

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Enquiries regarding purchase of the system should be made to the BMR Sales Centre at the same address (phone (06) 2499519, fax (06) 2576466).

# ABSTRACT

MDA (Mineral Data Analysis) is a comprehensive IBM PC-based system for processing mineral chemical data, particularly those obtained by electron probe microanalyser. It is designed to use mineral chemical data which may be entered into files from the keyboard, transferred from files generated on the microprobe, or retrieved from a database such as ORACLE. MDA is an extension of GDA (Geochemical Data Analysis), BMR's comprehensive PC-based system for processing whole-rock geochemical data. The programs are written in FORTRAN 77 (Microsoft compiler) and use the MicroGlyph Systems Sciplot graphics package for plotting. The system includes facilities for generating plots (histograms, XY plots, triangular plots, etc), calculating statistical functions (e.g., mean, standard deviation, regression lines, correlation coefficients and cluster analysis) as well as enabling calculation of end-member molecules, the classification and naming of minerals, and the printing of tables of analyses. Plots can be displayed on screen for inspection and editing before being output to a plotter or other device. Other programs allow samples to be assigned to groups for plotting purposes, and editing and merging of data files.

MDA is currently used at BMR to process all mineral chemical data obtained by electron probe micro-analyser for petrology-oriented research projects. The package could be readily employed in anyproject requiring manipulation of mineral analyses. It is likely to find particular application in the field of diamond exploration which relies heavily on the chemical discrimination of indicator minerals.

# CONTENTS

# LIST OF TABLES

# LIST OF FIGURES

# 1 INTRODUCTION

The mineral data analysis (MDA) system is an extension of the Bureau of Mineral Resources Geology and Geophysics (BMR) IBM PC-based geochemical data analysis (GDA) system to enable processing of mineral analyses obtained by electron probe microanalyser. It was developed by Lloyd Simons, a contract programmer with Liveware Computer Services, for BMR. The MDA system utilises many of the GDA programs which enable transfer of data from an Oracle database, processing, the generation of plots (histograms, XY plots, triangular plots, and box-whisker plots) and the calculation of statistical functions, but includes a number of programs which are specific to mineral chemical analyses. These programs permit entry of mineral analyses into files, the calculation of structural formulae, estimation of $Fe_2O_3$ and $Fe^{3+}$ content, calculation of end-member components, classification and naming of certain minerals, and specialised plots such as the spinel prism.

This manual is intended to explain the general operation of the system which is largely menu-driven. It should be read in conjunction with the GDA manual (BMR Record 1992/1) but the MDA system can be operated without prior experience or knowledge of GDA. For both systems a basic knowledge of IBM-compatible PCs and MS-DOS is assumed. A summary outlining the operation of the system is given in Section 13.

## 1.1 COMMAND SUMMARY

The MDA system comprises three main programs - ENTMIN, BMRMDA and TABMIN. MDA also uses eight other programs which are common to GDA and MDA. These are linked with the GDA programs for handling geochemical analyses into a common GDA-MDA starting menu shown below. The common menu is called by keying MDA (or GDA). Each of the programs can then be run by typing the appropriate number from the menu or the name of the program.

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

CLUSTER – Q- and R-mode cluster analysis with dendrogram output (comprises two programs - CLUSTA and BMRDEND).

BMRDEND – generates the dendrogram output from the cluster analysis program (CLUSTA).

ENTMIN – accepts mineral data entered from the keyboard and writes them out in Oracle format.

BMRMDA – the core program of MDA. This enables data to be extracted into datasets, either directly or using specified arithmetic expressions or standard operations (e.g., $Mg/(Mg+Fe^{2+})$); calculation of end-member components; classification and naming of minerals; plots of these datasets can be previewed on the PC screen and output to files for later plotting.

ORACLE – reads the ASCII file which is either created by keyboard entry or imported from a database (e.g., Oracle) and writes the data to an internal (GDA) file for subsequent processing.

OUTGDA – writes contents of a GDA file to an ASCII file for entry to a data base (e.g., ORACLE) or for export and/or processing by other systems.

VECTOR – outputs graphics files (from MDA and GDA) to a plotter or other device.

STATS – generates correlation matrices and sample statistics.

TABMIN – generates tables of analyses including major and trace elements, structural formulae, and cation ratios as required.

UTIL – utilities that allow editing of GDA files.

Users of the earlier versions of GDA and MDA, which utilised HALO graphics, should note that BMRGDA, BMRPMOD, BMRDEND and BMRMDA replace GDAPROG, PETMOD, DEND and MDAPROG respectively. However, both versions can be run on the same PC if required.

The GDA-MDA System is linked by a common menu run by the command MDA (or GDA) as follows:

**GEOCHEMICAL AND MINERAL DATA ANALYSIS**

*** COMMON PROGRAMS (GDA and MDA) ***

1 = Utility functions (UTIL)

2 = Convert from Oracle format (ASCII) file to GDA file (ORACLE)

3 = Assign samples to groups (ASSIGN)

4 = Output to plotter / printer (VECTOR)

5 = Statistical functions (STATS)

6 = Cluster analysis (CLUSTA)

7 = Dendrograms for cluster analysis (BMRDEND)

8 = Export GDA file as ASCII file (OUTGDA)

*** GEOCHEMICAL - GDA ONLY ***

9 = Geochemical data analysis (BMRGDA)

10 = Generate tables of analyses (TABLE)

11 = Petrological modelling (BMRPMOD)

*** MINERALS - MDA ONLY ***

12 = Enter mineral data from keyboard (ENTMIN)

13 = Minerals data analysis (BMRMDA)

14 = Generate tables of anlyses (TABMIN)

The TABLE program can be used for mineral data, but does not allow printing of structural formulae (see GDA manaual for further details)

## 1.2 PARAMETER FILES

System parameters, such as element to oxide conversion factors, are held on files which can be modified with a text editor or word processor (e.g., WORD STAR non-document mode). Some files are generated during processing and can also be modified. Care must be taken to preserve the format (logical struc ture) 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 generally the name of the program with extension .PRN (e.g., STATS.PRN, TABMIN.PRN), but MDA.PRN is the output file for BMRMDA. Such files can be edited in any way required, as they are not used by the MDA system.

## 1.4 USER INTERFACE

The programs are controlled by selection of options from menus at the system and program level 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.

Program menus are of the following form:

1 = Histogram

2 = XY plot

3 = Triangular plot

Q = Quit

Option (1-3, Q) (exit)

where the option is chosen by typing the related number (followed by Enter). In some cases a hierarchy of menus is presented; the Enter keystroke 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 [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 values that will be taken on the Enter keystroke are 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.

Any program can be terminated (aborted) by using the **CONTROL** and **C** keys to return to the operating system.

## 1.5 SOFTWARE

All the software is written in Microsoft FORTRAN 77 (version 4.1). Microglyph Systems Sciplot is used for graphics to provide support for HP plotters, dot matrix printers, laser printers and several displays (EGA, Hercules, CGA and VGA).

## 1.6 HARDWARE REQUIREMENTS

An IBM PC or compatible is required with 640K RAM, a 10 megabyte hard disk (the actual GDA and MDA programs require about 6 MB, and a Hercules, EGA, CGA or VGA colour graphics card. An HP compatible plotter is required for hardcopy graphics and a printer for reports (or monochrome graphics).

## 1.7 GDA FILE

Like the GDA system, MDA operates on sets of assigned 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 used in the standard definition files OXIDE.DEF and METAL.DEF include the analysis number, the mineral name, and number of cations and oxygens in the mineral formula. Descriptions can be up to 32 characters. The 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 for silicate and oxide minerals or elements for metals and sulphides) are given in weight percent, whereas 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 (a value of 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 include any information desired, but the sample number must have the name 'SAMPNO'; the analysis number (ANALNO) is optional, but will commonly be required, since there may well be a number of analyses from the same sample.

The data can be extracted from an existing database, transferred from EPMA in the form of an ASCII file or entered from keyboard using the program ENTMIN. All data 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 should be given names with the extension .GDA. It is recommended that the same Oracle file name be used with the GDA extension (e.g., BOWHILL.ORC and BOWHILL.GDA).

**NOTE:** The facility to list all Oracle-format and GDA files (by typing '?') when running programs requires the correct file extension.

Before data in a GDA file can be processed, samples must be assigned to groups using the ASSIGN program. After assignment of samples the various data-processing programs (BMRMDA, VECTOR, TABMIN, STATS, CLUSTER, etc.) can be used.

# 2 INSTALLATION

The MDA system requires the GDA system for its operation since many programs are common (however, GDA may be run without MDA). The software is provided on floppy disks in either 5.25" or 3.5" format, and is installed on the PC as follows:

- Set up a directory (normally \GDA\) on the hard disk by typing mkdir GDA;
- Copy the contents of all the floppy disks to this GDA directory; (if GDA is already on the hard disk, copy only the additional MDA programs and files);
- Edit the file SITE.DEF to specify the appropriate graphics card for your system (EGA or VGA). The HP plotter needs to be specified only for the versions of GDA and MDA which use the HALO graphics package. 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 Magenta
7    1.00 0.50 0.00 Brown
8    1.00 0.50 0.50 Light Red
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
```

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 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. For other output devices, the page size is set by the user when the BMRMDA program is run.

Three files in Oracle format, GARNET.ORC and AMPHIB.ORC (for oxide and silicate minerals) and SULPHIDE.ORC (for metals and sulphide minerals), are provided for use when trying out the system.

# 3 DATA ENTRY

Data may be entered into the MDA system by direct transfer from the EPMA via an ASCII file, from keyboard using the ENTMIN program, or by extraction from a database such as the BMR Oracle database.

## 3.1 FROM MICROPROBE (PROBE)

Data may be transferred directly from the electron probe microanalyser to the GDA/MDA system in the form of an ASCII file. Such a file must have a particular format, as described under ORACLE (see below).

## 3.2 FROM KEYBOARD (ENTMIN)

This program enables data to be entered from keyboard and is run by typing ENTMIN or nominating the appropriate option number (15) on the menu.

- The program first requires the name of the Oracle format file (e.g., BOWHILL.ORC). [Existing files with the extension .ORC may be listed by typing '?'].
- The mineral definition file must then be entered. OXIDE.DEF (the default option) is used for silicates and oxides, and METAL.DEF for metals and sulphides.
- The type of data to be entered – either oxides (as in silicates and oxide minerals) or elements (as in sulphides and metals) – must then be specified.
- The names of the oxides (or elements) to be entered must then be listed. These names must be identical to those listed on OXIDE.DEF(or METAL .DEF), or an error message will appear. However, the definition files can be edited to include extra oxides or elements. Note that SIO2 is automatically included as the first concentration field if it is not specified (e.g., for metals/sulphides). **15 is the maximum number of oxides or elements allowed in the file, or an error will result.**
- Data (normally in weight percentages) are then entered in turn until all the oxide or element fields are filled.

**NOTE:** If several sessions are required to enter a set of analyses, each session should use a different .ORC file as ENTMIN overwrites and does not append files of the same name. Files can be concatenated by using a text editor to join them (after appropriate edit) or by using the merge facility for GDA files under UTIL. When merging separate files under UTIL it is important that the sample entries have unique sample analysis numbers (SAMPNO/ANALNOs) to avoid confusion of sample numbers and ordering.

The following is an example of the commands and displays produced when ENTMIN is used to input a chromite analysis. Data are entered as oxides and the number of cations and oxygens in the ideal formula specified (3 cations per 4 oxygens in this case) to enable calculation of $Fe_2O_3$ and $Fe^{3+}$ contents from stoichiometry. Input data are indicated in following scheme by bold type.

C:\GDA>ENTMIN

ORACLE format file name [? = LIST]: **BOWHILL.ORC**

Mineral definitons file [? = LIST] (OXIDE.DEF): default

Enter oxides [Y/N=elements] (Y): default

give names of oxides to be entered

Oxide (exit): **SIO2**

Oxide (exit): **TIO2**

Oxide (exit): **AL2O3**

Oxide (exit): **CR2O3**

Oxide (exit): **V2O3**

Oxide (exit): **FEO**

Oxide (exit): **MNO**

Oxide (exit): **NIO**

Oxide (exit): **MGO**

Oxide (exit): **CAO**

Oxide (exit): default

Oxides/elements processed

MGO AL2O3 SIO2 CAO TIO2 V2O3 CR2O3 MNO FEO NIO

Enter values for next analysis

| | | |
|---|---|---|
| Wt % for SIO2 | (zero): | **.13** |
| Wt % for TIO2 | (zero): | **2.62** |
| Wt % for AL2O3 | (zero): | **3.32** |
| Wt % for CR2O3 | (zero): | **54.56** |
| Wt % for V2O3 | (zero): | **.07** |
| Wt % for FEO | (zero): | **32.68** |
| Wt % for MNO | (zero): | **.92** |
| Wt % for NIO | (zero): | **.06** |
| Wt % for MGO | (zero): | **5.46** |
| Wt % for CAO | (zero): | **.07** |

| | |
|---|---|
| Analysis no [1-10 chars]: | **38** |
| Sample number [1-10 chars]: | **83211078** |
| Mineral [1-32 chars]: | **CHROMITE** |

Mineral description [1-32 chars]: **GMASS, CORE, 20 MICRON GRAIN**

No cations for $Fe^{3+}$ calc. [0-99] **3**

Number oxygens **4.00**

| Analysis 83211078/38 | | GMASS, CORE, 20 MICRON GRAIN | |
|---|---|---|---|
| | wt % | O = 4 | ppm |
| MgO | 5.46 | 0.2853 | 32930 |
| Al2O3 | 3.32 | 0.1372 | 17571 |
| SiO2 | .13 | .0046 | 608 |
| CaO | .07 | .0026 | 500 |
| TiO2 | 2.62 | .0691 | 15707 |
| V2O3 | .07 | .0020 | 476 |
| Cr2O3 | 54.56 | 1.5122 | 373301 |
| MnO | .92 | .0273 | 7125 |
| Fe2O3 | 7.63 | .2014 | 53397 |
| FeO | 25.81 | .7567 | 200627 |
| NiO | .06 | .0017 | 472 |
| Total | 100.65 | 3.0000 | |

Normalise oxide concentrations [Y/N] (N)?

Oxide to change (none):

Analysis no 38

Sample no 83211078

Mineral CHROMITE

Description GMASS, CORE, 20 MICRON GRAIN

Number oxygens 4.00

Number cations 3

Change values [Y/N (N)?

Accept analysis [U/N] (Y):

Enter another analysis [Y/N] (Y)?

The output file is in ORACLE (i.e., ASCII) format, similar to those shown in section 4 (ORACLE).

## 3.3 FROM ORACLE DATABASE

Data may be extracted from a database, such as ORACLE, in ASCII format. Two examples of input files are given under ORACLE.

## 3.4 USING UTIL PROGRAM

Data may be entered directly into a GDA file using the UTIL program, although, unlike ENTMIN, this option does not display structural formulae as a check on the quality of the analyses when entering the data. There is, however, a separate operation (16) to display structural formulae and normalise mineral analyses. Procedures are described under UTIL (see below).

# 4 ORACLE

Data entered into the system in Oracle format ASCII files, including those generated using ENTMIN, but not those using UTIL, must be converted into internal (GDA) files for subsequent processing using the ORACLE program.

Data in ASCII format may be edited using a text editor (non-document mode in WORDSTAR) prior to conversion to an internal (GDA) file. Any data can be entered providing they are in this format, i.e., the Oracle database does not have to be used.

The file consists of records (i.e., lines) of up to 80 characters. 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. Two examples of ASCII files in Oracle format are given below.

The first contains analyses of garnets in rocks from theYilgarn Block. Note that concentration data are stored both as oxide weight percentages and element parts per million (ppm). This allows minor or trace elements to be processed using the more precise ppm data, but the input file does not have to be in this form (and commonly will contain only oxide weight percentages). The second example is for sulphides from the Munni Munni layered complex. In this case, only element weight percentages are included. The SIO2 field has been included (although there are no data) to define the first concentration (i.e., numerical) field.

```
YILGARN GARNET DATA

ANALNO
----------
SAMPNO
----------
MINERAL
--------------------------------
MINDESCR
--------------------------------
OXYGENS
----------
CATIONS
----------
SIO2
----------
NA2O
----------
MGO
----------
AL2O3
----------
K2O
----------
CAO
----------
TIO2
----------
CR2O3
----------
MNO
----------
```

```
FEO
----------
NIO
----------
NA
----------
MG
----------
AL
----------
SI
----------
K
----------
CA
----------
TI
----------
CR
----------
MN
----------
FE
----------
NI
----------
97288
91964546
garnet
large grain - core
 12.0
  8.0
   36.4833
     .0421
     .5589
   21.1642
    -.0107
     .3292
     .0537
    -.0399
   15.8251
   24.7835
    -.0789
     312.0
    3371.0
  112012.0
  170537.0
     -89.0
    2353.0
     322.0
    -273.0
  122559.0
  192646.0
    -620.0
97289
91964546
garnet
large grain - rim
 12.0
  8.0
```

```
   36.4649
    -.0263
     .5186
   21.1508
    -.0110
     .2852
     .0495
    -.0399
   16.3361
   25.8904
    -.0757
    -195.0
    3128.0
  111941.0
  170451.0
    -91.0
    2038.0
     297.0
    -273.0
  126517.0
  201250.0
    -595.0


MUNNI MUNNI SULPHIDES

ANALNO
----------
SAMPNO
----------
MINERAL
--------------------------------
MINDESCR
--------------------------------
OXYGENS
----------
CATIONS
----------
SIO2
----------
S
----------
FE
----------
CO
----------
NI
----------
CU
----------
ZN
----------
AS
----------
59794
84770102
pyrrhotite
fine intergrowth
   .0
   .0
```

```
      .0000
    37.4485
    60.0128
     -.0144
      .4491
      .0229
     -.0133
     -.0273
59795
84770102
pentlandite
small grain
    .0
    .0
      .0000
    31.0035
    30.7180
     4.4265
    33.9463
      .1179
      .0144
     -.0280
59796
84770102
chalcopyrite
intergrown with pyrrhotite
    .0
    .0
      .0000
    32.8055
    31.8457
      .0432
      .1836
    33.9222
     -.0135
     -.0281
```

Restrictions applying to the file 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 characters are usually enough for concentrations, but ten is 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 analysis.
- The field SAMPNO must be in the descriptive fields to give an identifier for each sample (for assigning purposes, etc.). The optional field ANALNO is usually used for mineral analyses as there are commonly 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 fields. 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.
- Note that ENTMIN automatically includes the SIO2 field, if it is not specified (e.g., for element sulphide analyses).
- 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 or option 2 of the main GDA-MDA menu.

You must provide the name of the Oracle file to be read in (e.g., WAND.ORC). [Typing '?' gives a list of existing .ORC files].

You must also give the name of the internal file to be generated. The default CURRENT.GDA is also the default for other programs. It is advisable to use the same file name for the GDA file as for the Oracle file, with the respec tive .GDA and .ORC extensions.

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.

The file FIX.DEF is used to change the names of the concentration fields on the file, although this will not normally be necessary unless the input (ASCII) contains non-standard names (e.g., water, rather than H2O).

# 5 ASSIGN

As with GDA 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 so that all samples within it are represented by the same symbol and pen colour. At least some of the samples on a GDA file must be assigned to groups (or a single group) before plots can be generated.

Samples are assigned to a group according to logical operations on the descriptive fields (e.g., SAMPNO, ANALNO, MINERAL, MINDESCR, etc.) on the file.

The program is run by typing ASSIGN or option 3 on the main GDA-MDA menu. Option 1 on the ASSIGN menu is then selected to define the group logic. A global selection can be specified to provide overall criteria for accepting or rejecting samples in up to 10 lines (logical 'or' conditions); if no global logic is specified all samples will be considered.

The following must be specified for each group:

- The group name (maximum of 20 characters), which appears on the legend and on menus for selection of group parameters such as the symbol;
- Logical expressions to assign samples to the group.

The logic is typed in as lines, where each line is an 'or' condition. A maximum of 10 lines (i.e., conditions) 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, different minerals can be assigned to separate groups using MINERAL == or different groups of the same mineral assigned to separate groups on the basis of mineral description using MINDESC == , rock type using LITHOLOGY == , or rock unit using STRATUNIT = = , etc.

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 extra information in other fields (e.g., OTHERDATA) to aid assignment of samples or analyses into groups.

After the logic has been specified for each group the file is processed and the samples assigned to groups (option 12). Where the assignment criteria are ambiguous or a sample(s) has characteristics found in more than one group it will be assigned to the first group encountered and the other assignable groups listed as 'group conflict'. Samples falling outside the assignment criteria are not assigned. 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 ASSIGN 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 text editor or 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 reassigned 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 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

(Q) Quit

An example of a logic file (for heavy minerals in concentrate from the Wandagee alkaline ultrabasic suite) is given below. This logic will extract chromites from Wandagee pipe M97 into group 1, all other Wandagee chromites into group 2, Wandagee pipe M89 garnets into group 3 and all other Wandagee garnets into group 4.

Global logic

SAMPNO == WANDAGEE

Group number 1

PIPE M97 CHROMITES

MINERAL == CHROMITE && STRATUNIT == PIPE M97

Group number 2

WANDAGEE CHROMITES

MINERAL == CHROMITE

Group number 3

PIPE M89 GARNETS

MINERAL == GARNET && STRATUNIT == PIPE M89

Group number 4

WANDAGEE GARNETS

MINERAL == GARNET

The assignment of samples into the specified groups may be printed out from the file ASSIGN.PRN.

# 6 BMRMDA

This is the main program or core of MDA. It allows data to be extracted and plotted on various types of graph (XY, XYZ, histogram, box-whisker, etc).

Data may be extracted on the basis of oxide/element concentration, structural formula (i.e., cations), atomic ratios or, for particular minerals such as pyroxenes, amphiboles, spinels and garnets, as the percentage of end-member components. Options allow printing of specialised reports for these minerals which allocate cations, calculate end-member components, and name and/or classify the mineral. Another option allows projection of spinel compositions into the spinel prism.

The MDA program is run by typing BMRMDA or option 13 on the main GDA-MDA menu. A GDA file name (as generated in the ORACLE program) must be specified (if using a floppy disc the drive must be specified eg., A:\xyz). The output graphics device (i.e., file type) is then selected from:

1 = Plotter metafile

2 = Printer metafile

3 = Postscript Ascii file

4 = Encapsulated Postscript file

5 = HPGL file

6 = CGM file

7 = WordPerfect graphics file

Plot files generated in BMRMDA are output using the VECTOR program (see below), although some types may be copied directly to printers or other devices. The plotter metafile is for output to pen plotters, the printer metafile for dot matrix printers, and the remainder for laser printers or word processors (see under VECTOR for more details). The plotter and printer metafiles are virtually identical (although the default plot sizes are different) and either may be displayed on screen using VECTOR.

The device width determines the size of the final plot, and the default values are selected to give a full size (normally 25 x 20cm) plot on a pen plotter (using A3 paper) and a half-scale (12.5 X 10cm) plot on dot matrix and laser printers and other plot file types. However, these sizes may vary, depending on the actual plotter/printer used.

The line width determines the line thickness of the final plot. However, this does not apply to pen plotters or HPGL or Wordperfect graphics files.

Finally, the mineral definition file, either OXIDE.DEF or METAL.DEF, depending on whether the data are as oxide or element concentrations, must be given.

The MDA menu will then appear as follows:

MINERALS

(1) Extract values for typed in expressions

(2) Extract structural formulae into data sets

(3) Extract pyroxenes into data sets

(4) Extract amphiboles into data sets

(5) Extract spinels into data sets

(6) Extract garnets into data sets

(7) Select groups for display

(8) Delete all plot files

(9) Define main plot parameters

(10) Display data sets

(11) Display histograms

(12) Display XY plot

(13) Display triangular plot

(14) Display legend

(15) Display spinel prism

(16) Display box-whisker plot

(17) Print structural formulae report

(18) Print pyroxenes report

(19) Print amphiboles report

(20) Print amphibole classification report

(21) Print spinels report

(22) Print garnets report

(23) Specify a different GDA file

(Q) Quit

Option (1-23, Q):

In the above menu, items 1 - 16 relate to extraction from GDA files and graphical presentation of data. The data can be displayed on screen and/or written to a plot file (GDA1.VEC, etc.) for plotting by pen plotter or laser printer. Items 17 - 22 are programs for the calculation of structural formulae and printing of analyses, structural formulae, cation ratios, end-member components, and the mineral classification. In these

applications the output is to the print file MDA.PRN which may be edited by text-editor or word processor prior to printing.

For graphical display/analysis the first step is to extract data, either the stored oxide/element concentrations or information calculated from these, such as cations, end-member components, cation ratios, etc., from the GDA file for plotting. Data are extracted into datasets (up to 4) using items 1 - 6.

Data extracted into datasets can be plotted on various diagrams, namely datasets display, histograms, XY plots, triangular plots, box-whisker plots, and the reduced and oxidised spinel prisms. Plot legends (i.e., symbols and group names) may also be displayed. These options are called up using items 10 - 14 on the MDA menu. Text may be added to any plot, and some types of plot include statistical functions such as regression lines, means, and standard deviations, which may be displayed if required. A shortage of memory precludes calculation of least-squares lines for MDA. Regression curves are available, but note that these assume that there are no errors in the X-axis variable, i.e., X is the independent variable and Y the dependent variable. Normally, plots are intially displayed on the PC screen to allow inspection and editing before being written to metafiles for later output to a plotter using the VECTOR program. Examples of the various plots available are shown below in the relevant sections.

## 6.1 EXTRACT VALUES FOR TYPED - IN EXPRESSIONS

This option is used to extract oxide or element abundances and other information such as stratigraphic height or isotopic composition, stored in the specified GDA file and any derived values formed by arithmetic combination of the oxide/element concentrations or other numerical data stored. It does *not* enable extraction of cations from structural formulae (options 2 - 6 apply).

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 |

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.

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

The following example extracts from a set of chromite analyses the $Cr_2O_3$ and MgO contents (datasets 1 and 2), the $Al_2O_3$ + $Fe_2O_3$ content (dataset 3) and $Cr_2O_3$ values for chromites with more than 56% $Cr_2O_3$ (dataset 4).

Entered responses are in bold type.

Type arithmetic expression [?=help] (Exit)

**: CR203**

Data set number [1 - 4]: **1**

Type arithmetic expression [?=help] (Exit)

**: MGO**

Data set number [1 4 ]: **2**

Type arithmetic expression [?-help] (Exit)

**: AL203 +Fe203**

Data set number [1 - 4]: **3**

Type arithmetic expression [?=help] (Exit)

**: CR203 >56**

Data set number [1 - 4]: **4**

These datasets can be displayed using option 10 (= Display datasets) followed by the DATASET sub-menu options 1 and 2. Datasets selected are used as the X axis.

A help file is available by returning **?**

The help file also lists the oxides and/or element names held in the GDA file which can be extracted.

Derived values are formed from arithmetic combinations of element or oxide concentrations. Components are identified by name.

An example is:

(FE2O3+FEO)/2 >50 <90.0

This creates a new concentration which is half the sum of the concentrations of the individual components (in this case oxides). Any valid arithmetic expression is permitted, but only values in the given range are accepted. Previously calculated values held in other datasets can be referenced by using the two characters $n, where n is the dataset number. This enables holding of intermediate values in datasets.

Press Enter to continue.

## 6.2 EXTRACT STRUCTURAL FORMULAE INTO DATASETS

This option is used to extract cations (or any arithmetic combination of cations) calculated from the oxide and element concentrations in the GDA file. The program calculates structural formulae on the basis of the number of oxygens specified in the GDA file. An option is available to specify calculation with or without ferric iron, but note that ferric iron can only be calculated if both oxygen and cation numbers are given on the GDA file.

The following is an example of the type of cation ratios commonly used in plotting of chromian spinels.

Calculate Ferric [Y/N] (N)? **Y**

Type arithmetic expression [?=help] (Exit)

**: 100*Cr/(Cr+Al)**

Dataset number [1 - 4]: **1**

Type arithmetic expression [?=help] (Exit)

**: 100*Mg/(Mg+Fe2+)**

Dataset number [1 - 4]: **2**

Type arithmetic expression [?=help] (Exit)

**: Fe3+/(Cr+Al+Fe3+)**

Dataset number [1 - 4]: **3**

Type arithmetic expression [?=help] (Exit)

**: Cr/(Cr+Al+Fe3+)**

Dataset number [1 - 4]: **4**

The calculation of ferric takes slightly longer to perform than the standard structural formula.

Atomic ratios such as 100K/(K+Na+Ca) (i.e., Or content), can be extracted and later renamed (in this example to 'Mol percent Or') using options provided under the plotting routines.

Extraction of combined oxide or element weight percent data, or other parameters, such as stratigraphic height or structural formulae components, can be made by sequential extraction using options 1 and 2 and storing the data as datasets 1-4. Data from previous extractions will be held in their designated datasets until overwritten by subsequent extractions or exit from the BMRMDA program.

## 6.3 EXTRACT PYROXENES INTO DATASETS

This option extracts pyroxenes and calculates structural formulae on the basis of 6 oxygen atoms, estimates $Fe^{3+}$ assuming pyroxene stoichiometry (4 cations per 6 oxygen atoms), assigns cations to the various pyroxene sites (T, M1 and M2) and calculates ln activity $Mg_2Si_2O_6$, following the method of Wood and Banno (1973).

Atomic ratios are calculated as follows:

| | | |
|---|---|---|
| Mg# | = | $100Mg/(Mg+Fe^{2+})$ |
| Ca* | = | 100Ca/(Ca+Mg+Fe) |
| Mg* | = | 100Mg/(Ca+Mg+Fe) |
| Fe* | = | 100Fe/(Ca+Mg+Fe) |
| WO" | = | 100Wo/(Wo+En+Fs) |
| EN" | = | 100En/(Wo+En+Fs) |
| FS" | = | 100Fs/(Wo+En+Fs) |
| ACF2 | = | $Al(Ml)+Cr+Fe^{3+}+2Ti$ |
| ln(a)En | = | log activity enstatite |

Wo, En and Fs are calculated after the other end-members in the order given below.

The program also calculates the molecular percentage of the end members:

| | | |
|---|---|---|
| $NaCrSi_2O_6$ | (Ureyite) | Ur |
| $CaCr_2SiO_6$ | (Ca-Cr-tschermaks) | CaCrTs |
| $NaAlSi_2O_6$ | (Jadeite) | Jd |
| $NaFe^{3+}Si_2O_6$ | (Acmite) | Ac |
| $CaTiAl_2O_6$ | (Ca-Ti-tschermaks) | CaTiTs |
| $CaAl_2SiO_6$ | (Ca-tschermaks) | CaTs |
| $CaFe^{3+}{}_2SiO_6$ | (Ca-ferritschermaks) | CaFeTs |
| $CaSiO_3$ | (Wollastonite) | Wo |
| $MgSiO_3$ | (Enstatite) | En |
| $FeSiO_3$ | (Ferrosilite) | Fs |

End-members are calculated in the order listed following the method of Cawthorn and Collerson (1974), except that the Cr pyroxene components ureyite and Ca-Cr-tschermaks are calculated before jadeite.

The full list of cations, site allocations, atomic percentages and molecular percentages of end-members, displayed under [?] help, is:

| | | | | | | |
|---|---|---|---|---|---|---|
| Si | Ti | Al | Cr | Fe3+ | Fe2+ | Mn |
| Ni | Mg | Ca | Na | K | Sum | Al/2 |
| Al(T) | Al(Ml) | Mg(Ml) | (ACF2T) | T(tot) | Ml(tot) | M2(tot) |
| ln(a)EN | mg# | Ca* | Mg* | Fe* | WO" | EN" |
| FS" | Ur | CaCrTs | Ac | Jd | CaTiTs | CaTs |
| CaFeTs | Wo | En | Fs | | | |

This can be viewed by selecting the help option (?) when asked to type arithmetic expression. Derived values may be formed by any arithmetic combination of the above values.

## 6.4 EXTRACT AMPHIBOLES INTO DATASETS

This option extracts data from the GDA file and calculates structural formulae, as well as amphibole base end-members (Mol%) and site allocations. Estimation of ferric iron is by normalising cations exclusive of Ca, Na, and K to 13, i.e., T + C = 13 (when Ca+Na> 1.34), or by normalising the T + C + B exclusive of Na and K to 15 cations (when Ca+Na> 1.34). The first option is generally preferable for most amphiboles, particularly calciferous ones, whereas the normalisation to T + C + B = 15 is preferable for the anthophyllite - cummingtonite series.

Element names are:

| | | | | | | |
|---|---|---|---|---|---|---|
| Si | Ti | Al | Cr | Fe3+ | Fe2+ | Mn |
| Ni | Zn | Mg | Ca | Na | K | Al4 |
| Al6 | FMM1 | FMM4 | CaM4 | NaM4 | NaA | ATot |
| Mg# | Fe3# | Ca" | Mg" | Fe2" | Anth | Gedrite |
| Tremolite | Hornblende | Tschermak | Winchite | Barroisite | Rieb+Glauc | Na-anth |
| Na-Gedrite | Edenite | Parg+Hast | Richterite | Kataphor | Taramite | Arfv+Eck |
| Nyboite | Kaersutite | | | | | |

where Al4 and Al6 refer to tetrahedral and octahedral Al, respectively, FMM1 and FMM4 are the sum of the ferromagnesian ($Fe^{2+}$+Mg+Mn+Ni+Zn) cations in the M1 and M4, sites respectively, and NaA is the number of Na cations in the A site.

$$Mg\# = 100\,Mg/(Mg+Fe^{2+})$$
$$Fe3\# = 100Fe^{3+}/(Fe^{2+}+Fe^{3+})$$
$$Ca" = 100Ca/(Ca+Mg+Fe^{2+})$$
$$Mg" = 100Mg/(Ca+Mg+Fe^{2+})$$
$$Fe" = 100Fe^{2+}/(Ca+Mg+Fe^{2+})$$

and the end-member names refer to ideal end-member amphiboles.

Calculation of the amphibole end-members is based on the method of Currie (1991).

Amphiboles have the general formula $A_{1-2}B_2C_5T_8O_{22}(OH,Cl,F)_2$ where A = Na, K; B = Na, Li, Ca, Mn, Mg, $Fe^{2+}$; C = Mg, $Fe^{2+}$, Mn, Al, $Fe^{3+}$, Ti ; T = Si, Al with other less

common substitutions. The A, B and T-sites are used to classify 17 end-member molecules (Hawthorne, 1983). Amphibole end-members are first classified into A-site empty and A-site full types. End-members are then calculated according to $Si_6$, $Si_7$ and $Si_8$ and B-site occupancy, with the B-site filled by FM, Ca or Na or mixed Na-Ca cations.

## 6.5 EXTRACT SPINELS INTO DATASETS

In this option spinels are extracted and their structural formulae are calculated on the basis of 4 oxygen atoms. Ideal end-member spinels are also calculated in the order listed following a modified version of the method of Mitchell and Clarke (1976). An option allows calculation of ferric iron assuming stoichiometry (i.e., 3 cations per 4 oxygens), depending on whether the oxidised or reduced spinel prism is selected.

For the oxidised prism the program calculates the following components (viewed using the help option).

Element names are:

| | | | | | | |
|---|---|---|---|---|---|---|
| Mg# | Al/TriV | Cr/TriV | Fe3+/TriV | Cr/(Cr+Al) | SI | TI |
| AL | CR | FE3+ | FE2+ | MN | MG | NB |
| V | NI | ZN | CA | ZnAl2O4 | MgAl2O4 | FeAl2O4 |
| MnAl2O4 | Mg2TiO4 | Mn2TiO4 | Fe2TiO4 | MgCr2O4 | FeCr2O4 | MnCr2O4 |
| Fe3O4 | | | | | | |

where TriV = the sum of the trivalent cations $(Al+Cr+Fe^{3+})/100$.

For the reduced spinel prism only the following components are calculated, endmembers, apart from Fe3O4, being essentially the same (prior to normalisation)

Element names are:

| | | | | | | |
|---|---|---|---|---|---|---|
| Mg# | Al/TriV | Cr/TriV | 2Ti/TriV | Cr/(Cr+Al) | SI | TI |
| AL | CR | FE2+ | MN | MG | NB | V |
| NI | ZN | CA | | | | |

where TriV = the sum of the tri-and quadrivalent cations (Al+Cr+2Ti)/100

## 6.6 EXTRACT GARNETS INTO DATASETS

This option allows garnet data to be extracted and structural formulae calculated on the basis of 12 oxygen atoms. Calculation of ferric iron assumes stoichiometry (8 cations per 12 oxygens). Selection can be made from concentration data, cations, cations in various sites, and end-member garnet molecules as shown in the listing below (viewed using the help option).

Element names are:

| | | | | | | |
|---|---|---|---|---|---|---|
| P2O5 | ZrO2 | SiO2 | TiO2 | Al2O3 | Cr2O3 | V2O3 |
| Y2O3 | Fe2O3 | FeO | MnO | NiO | MgO | CaO |
| Na2O | Total | P | Zr | Si | Ti | Al |
| Cr | V | Y | Fe3+ | Fe2+ | Mn | Ni |

| | | | | | | |
|---|---|---|---|---|---|---|
| Mg | Ca | Na | Sum | Ca* | Mg* | Fe* |
| MgNo# | MgNo | SiTET | AlTET | TiTET | Fe3+TET | SUM |
| SiY | AlY | Fe3Y | TiY | Y-Site | X-Site | Maj |
| Yt | Ya | Gold | Kimz | Fe-Kimz | Uvar | Knor |
| Sch | And | Py | Sp | Gr | Alm | Koh |
| Ski | Cal | Bly | | | | |

Calculation of the garnet end-members is modified from the method of Rickwood (1968) to include majorite (maj). The full names and formulae of the end-members are given in 6.21. MgNo# and MgNo refer to $100Mg/(Mg+Fe^{2+})$ calculated with FeO only and all Fe as FeO, respectively. Ca*, Mg*, and Fe* = $100\ Ca/(Ca+Mg+Fe^{2+})$, etc.

## 6.7 SELECT GROUPS FOR DISPLAY

This item allows selection of individual groups of samples within the data file.

Each of the groups is displayed in turn and selection is by responding yes or no.

## 6.8 DELETE ALL PLOT FILES

All existing plot files (GDA1.VEC etc.) are deleted by this function. Care should be taken to ensure that a back-up copy is made of those plot files required for future plotting (replotting).

## 6.9 DEFINING PLOT PARAMETERS

Item 9 on the MDA 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.

MAIN PLOT PARAMETERS

(1) Retrieve plot parameters (from file)

(2) Change title text height (1.5cm)

(3) Change axes labels text height (1.0cm)

(4) Change sample numbers and points text height

(5) Change symbol height (0.5cm)

(6) Change axes tick height (1.0cm)

(7) Change font (0.5)

(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 heights (1.0)

(16) Change axes lengths (X = 25.0cm; Y = 20.0cm)

(17) Define metafile path & preceding characters in name

(18) Store plot parameters (on file)

Option [1 - 17] (Exit):

An example of a plot parameters file is given in the GDA manual. Normally the format will not be of interest to the user as it will not be necessary to edit such a file.

There are choices of up to 8 pens (depending on the type of plotter), 15 symbols, 6 linetypes and 15 fonts (15 - 19 are the same), all of which may be displayed on screen by selecting the display option (?). 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. The default linetype for all groups is 1 (solid line); note that the linetypes as displayed on the screen may be slightly different from those used by the plotter.

The symbols, linetypes and fonts are shown in Figures 1-4 in the GDA manual.

The default axis lengths (25 x 20cm) produce a plot of that size on the plotter, and a 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 28cm 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 VECTOR). The default symbol and text sizes are appropriate for standard size plots, but may need changing if the axis lengths are greatly changed. 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.

Item 17 (define metafile path and preceding characters in name) allows plot metafiles to be written to a different drive (such as a floppy disk) or directory. The latter may be useful for a networked system. The specified path is added to the beginning of the plotfile name, but take care not to specify a non-existent directory. For example:

- C:\xxx\ would write the metafile to directory xxx on drive C (e.g., C:\xxx\GDA1.VEC);
- A: (or A:\) would write the metafile to floppy disk drive A (e.g., A:\GDA1.VEC);
- AB would add AB to the metafile name (e.g., ABGDA1.VEC);
- D:\GDB\AB would write the metafile to directory GDB on drive D and add the prefix AB (e.g., D:\GDB\ABGDA1.VEC).

The default is set so that the metafile is written to the current (i.e., GDA) directory.

## 6.10 DISPLAY DATASETS

This option 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 4 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 se lected 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 (0): (1 of up to 8 colours; displays mean for all groups selected for display in 13)

(11) Define pen for median lines (0) (as 10)

(12) Define pen for standard deviation lines (0)(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:

- 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)
- Pen number
- Symbol number (if none is given, only text will be output)
- Text (e.g., sample number or a legend; 0 - 50 characters)
- 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 MDA.PRN, which may subsequently be printed (and edited if required)

## 6.11 DISPLAY HISTOGRAMS

Histograms of three types may be displayed - for single datasets, stacked for up to 4 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

- Single element (for selected groups)
- Stacked for selected datasets (for all selected groups)
- 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):

- X, Y co-ordinates (separated by a comma; if no values are entered, previously specified points or text will be deleted)
- Pen number
- Symbol number (if none is given, only text will be output)
- Text (e.g., a legend; 0 - 50 characters)
- 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: 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 MDA.PRN).

An example of a histogram used to portray garnet compositions from two of the Wandagee alkaline ultrabasic pipes in Figure 1.

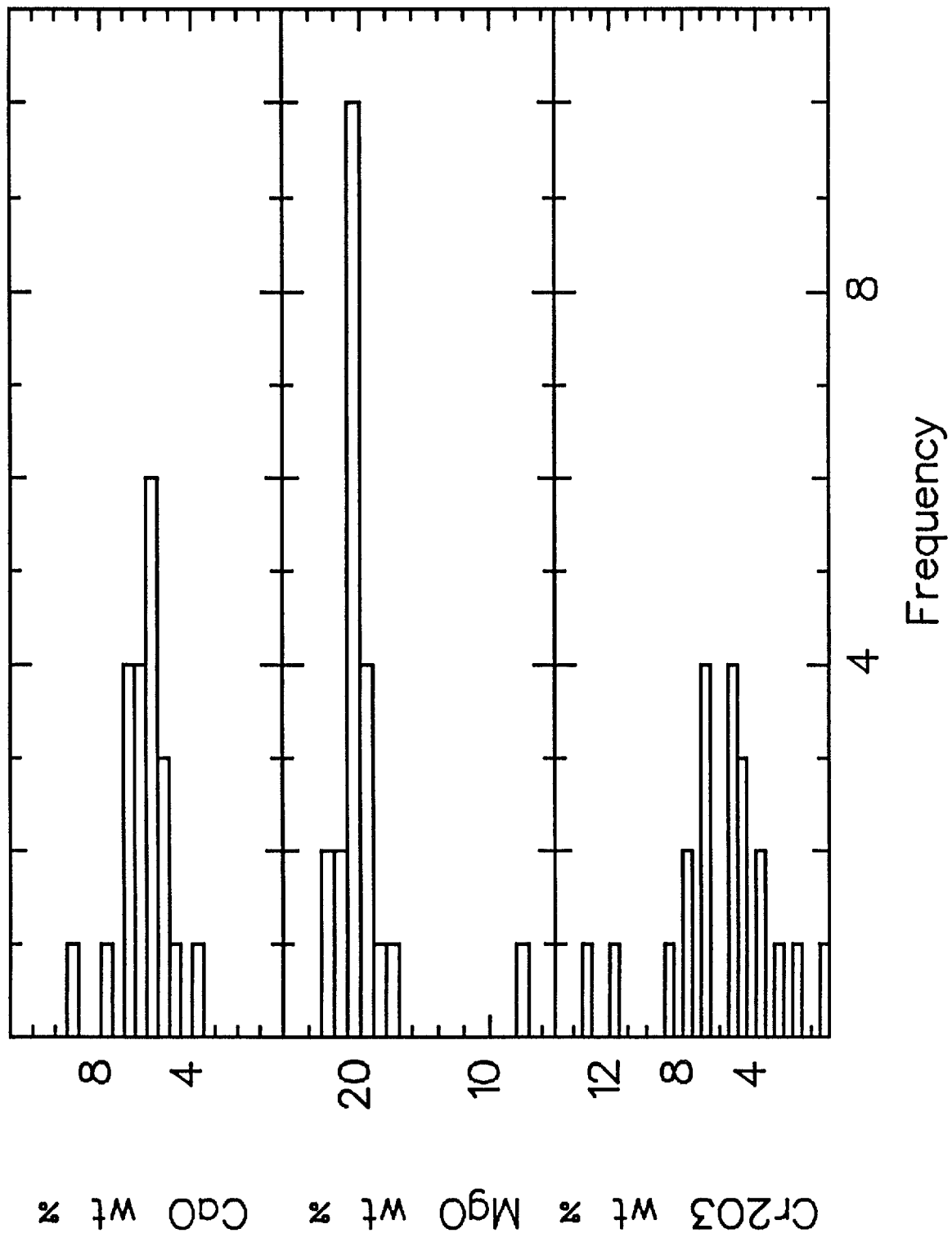


FIG. 1. STACKED HISTOGRAM OF GARNET COMPOSITIONS
Frequency
4
8
Cr2O3 wt %
8
4
MgO wt %
20
10
CaO wt %
12
8
4

## 6.12 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. Because of memory limitations options 13 and 19 on the GDA menu - least squares line fitting and least squares lines for individual groups are not available for MDA. The remainder are as follows:

(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

- X, Y co-ordinates (separated by a comma; previously specified points or text will be deleted if no values are entered here)
- Pen number
- Symbol number (if none given, only text will be output)
- Text (e.g., sample number or a legend; 0 - 50 characters)
- 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: 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).

Specify graphics overlay files (lines and/or text may be added by selecting an appropriate file - see appendix C 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)

(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 MDA.PRN)

An example of an XY plot showing the composition of diamond facies chrome spinels is shown in Figure 2 and the corresponding statistics printout is given in Table 1.

TABLE 1. STATISTICAL DATA FOR FIGURE 2.

XY PLOT OF DIAMOND FACIES CHROMITES

100Mg/(Mg+Fe2+)

| | |
|---|---|
| Minimum: | 2.8740 |
| Maximum: | 79.4540 |
| Mean: | 60.6240 |
| Median | 62.6530 |
| Standard Deviation: | 14.8066 |
| Skewness: | -1.8929 |
| Kurtosis: | 5.4445 |

100Cr/(Cr+Al)

| | |
|---|---|
| Minimum: | 82.8660 |
| Maximum: | 95.7810 |
| Mean: | 89.0946 |
| Median | 88.7500 |
| Standard Deviation: | 2.8370 |
| Skewness: | .4491 |
| Kurtosis: | .3798 |

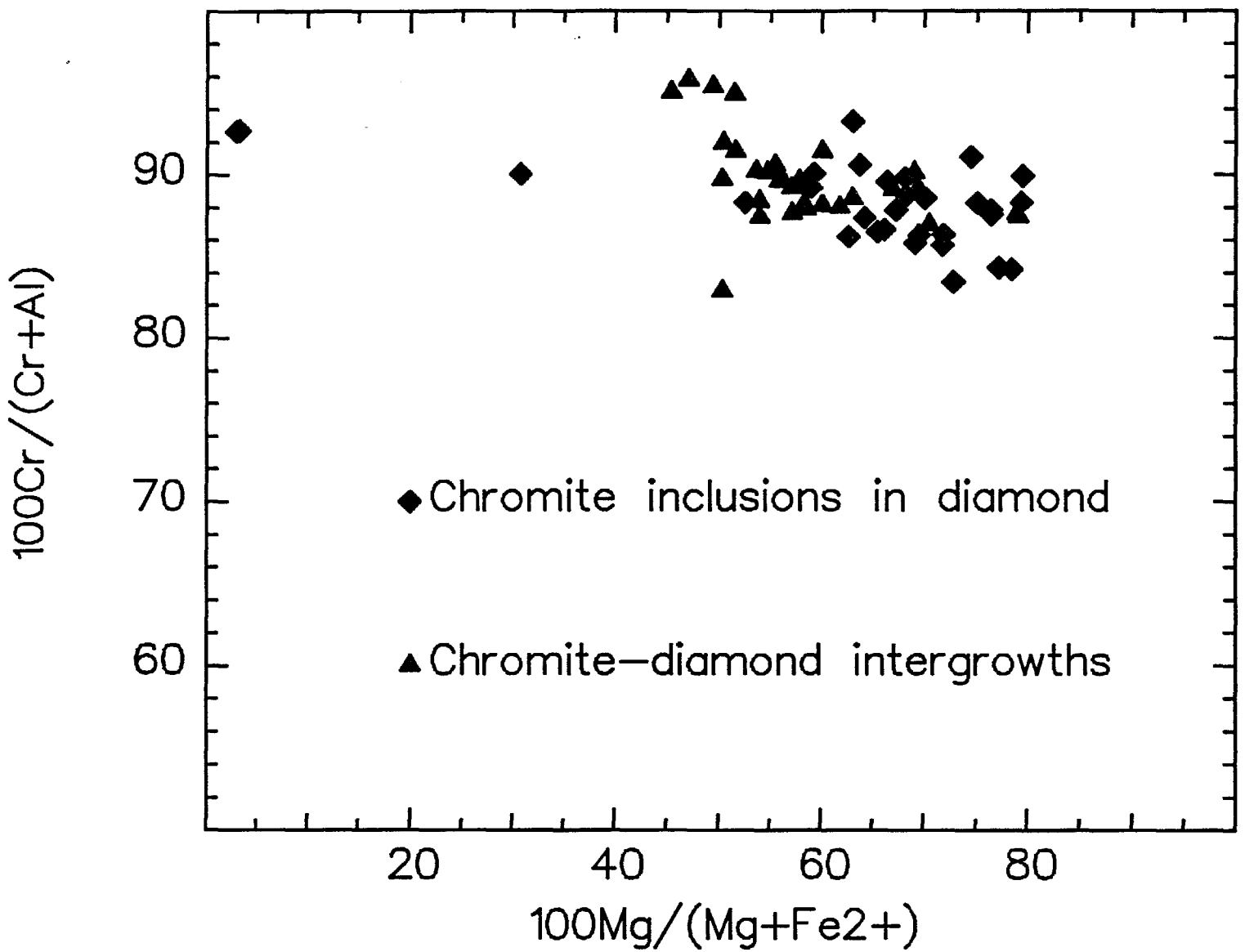
Regression Statistics:

Independent Variable: 100Mg/(Mg+Fe2+)
Dependent Variable: 100Cr/(Cr+Al)

Correlation Coefficient: -.5204
Product-Moment Correlation Coefficient
based on 61 pairs of values: -.5204

| | | | | |
|---|---|---|---|---|
| Polynomial of degree 1 | Standard error: | 2.4 | | |
| Regression Coefficient(s): | | 95.14 | -.9972E-01 | |
| Coefficient(s) Standard Deviation: | | .2130E-01 | | |
| T-Value(s): | | -4.682 | | |
| Polynomial of degree 2 | Standard error: | 2.4 | | |
| Regression Coefficient(s): | | 92.92 | .1701E-01 | -.1249E-02 |
| Coefficient(s) Standard Deviation: | | .7103E-01 | .7262E-03 | |
| T-Value(s): | | .2396 | -1.720 | |
| Polynomial of degree 3 | Standard error: | 2.4 | | |
| Regression Coefficient(s): | | 91.45 | .3589 | -.1103E-01 .7340E-04 |
| Coefficient(s) Standard Deviation: | | .2437 | .6711E-02 | .5009E-04 |
| T-Value(s): | | 1.473 | -1.643 | 1.465 |

FIG. 2. XY PLOT OF DIAMOND FACIES CHROMITES



## 6.13 DISPLAY TRIANGULAR PLOT

Any 3 datasets may be selected for display on a triangular plot.

(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

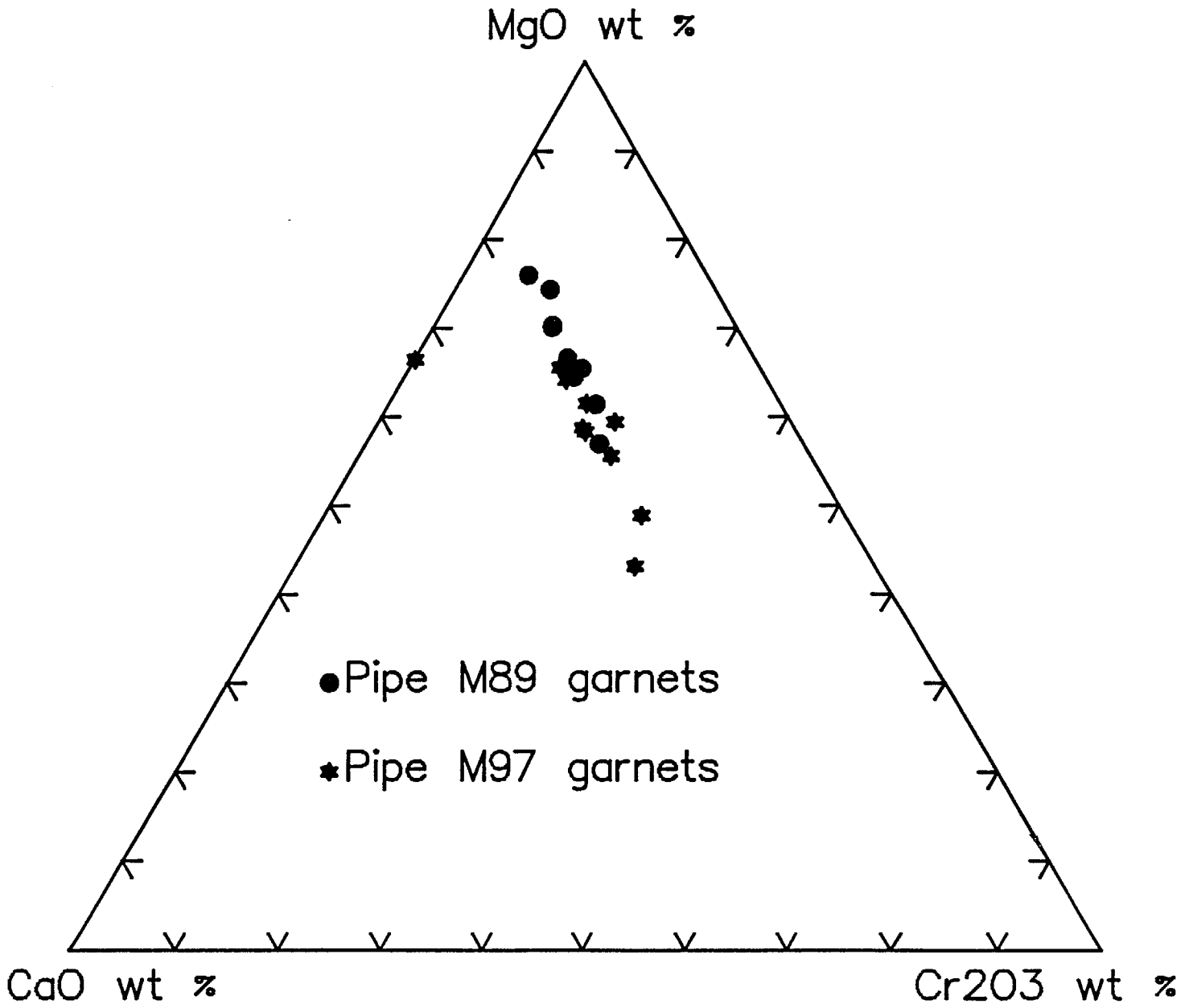
(7) Specify additional plot points and/or text (additional plot points or text, such as a legend, may be added to previously selected plots via the keyboard; the following must be given:

- 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 areas (i.e., negative) are permissible, but obviously must be adjacent to the plot)
- Pen number
- Symbol number (if none is given, only text will be output)
- Text (e.g., sample number or a legend; 0 - 50 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 units each).

(8) Specify graphics overlay files (xxx.GRF)

An example of a triangular plot showing the composition of garnets from two of the Wandagee alkaline ultrabasic pipes is given in Figure 3.

FIG. 3. XYZ PLOT OF GARNET COMPOSITIONS



## 6.14 DISPLAY LEGEND

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

## 6.15 DISPLAY SPINEL PRISM

This option allows spinel compositions to be plotted in the spinel prism (Irvine, 1965). Projections can be made into either the oxidised prism in terms of (MgFe)$Al_2O_4$-(MgFe)$Cr_2O_4$-(MgFe)$Fe_2O_4$ with $Fe^{3+}$ calculated from stoichiometry or the reduced prism in terms of (MgFe)$Al_2O_4$-(MgFe)$Cr_2O_4$-(MgFe)$_2TiO_4$ with all Fe assumed to be $Fe^{2+}$. The latter is useful for kimberlite spinels which formed under relatively reducing conditions.

The submenu is

SPINEL PRISM

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

(2) Change plot title

(3) Display sample numbers

(4) Select groups to be displayed

Examples of the spinel prism plots for both the oxidising and reduced prisms are shown in Figure 4. Note that for the oxidised prism, the symbol size is scaled according to the TiO2 content of the spinel: spinels with higher TiO2 contents are plotted using smaller symbols, because such compositions generally occur in more evolved rocks and are relatively fine-grained.

FIG. 4A. OXIDISED SPINEL PRISM PLOT

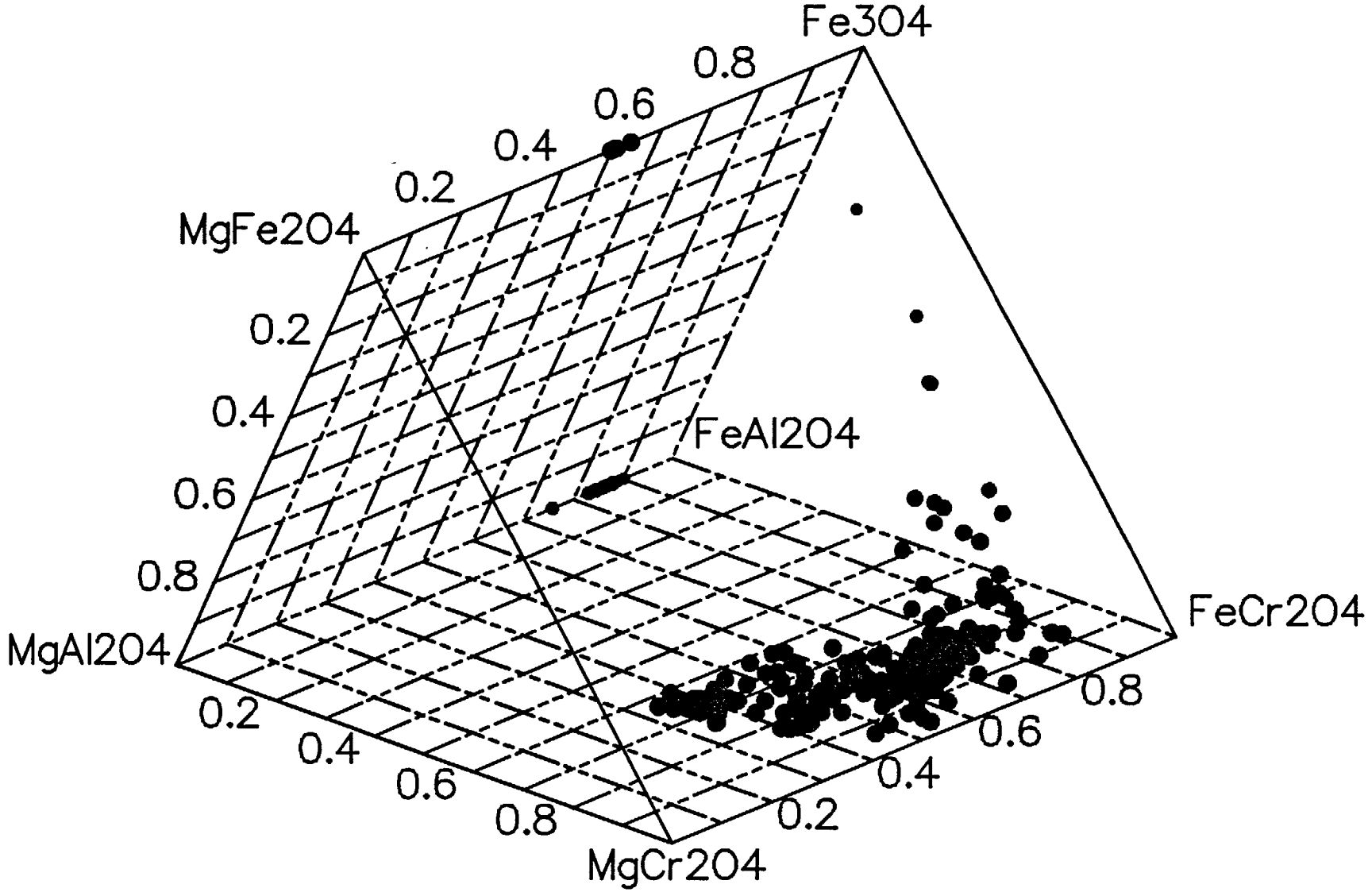
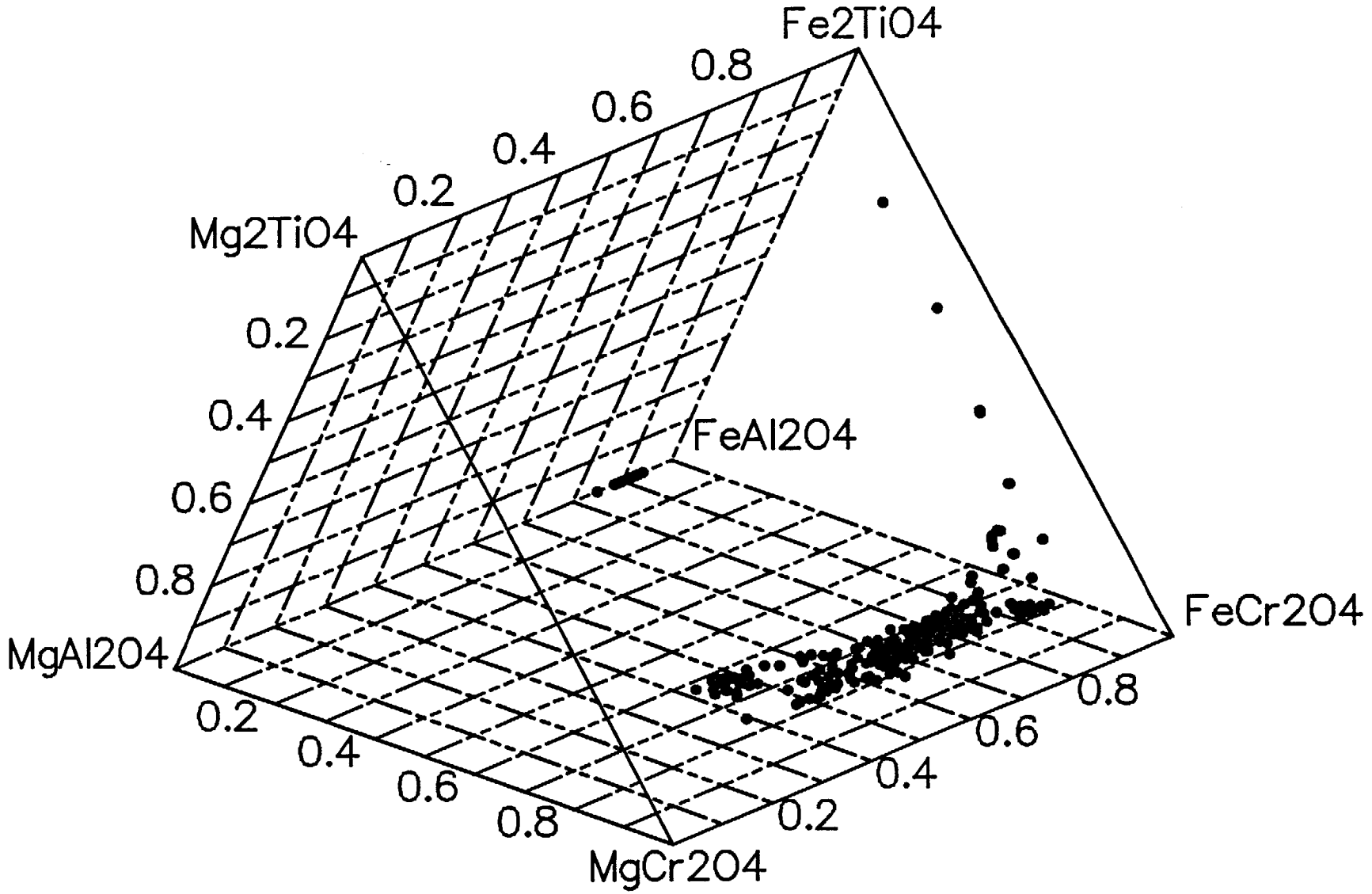


FIG. 4B. REDUCED SPINEL PRISM PLOT



## 6.16 DISPLAY BOX-WHISKER PLOT

Box-whisker plots may be used to display many datasets on a single diagram together with mean and standard deviation boxes for each dataset. Such plots are useful for highlighting anomalous values and for making comparisons with average data. The box-whisker menu is:

BOX-WHISKER PLOT

(1) Display

(2) Change plot title

(3) Set axes extremes to data range plus 20%

(4) Set axes extremes to nice limits

(5) Set axes extremes to typed in values

(6) Select groups to be displayed

(7) Select box-whisker type

(8) Specify additional plot points and/or text

(9) Specify box size

(10) Display box

(11) Display samples inside box

(12) Linear / log axis

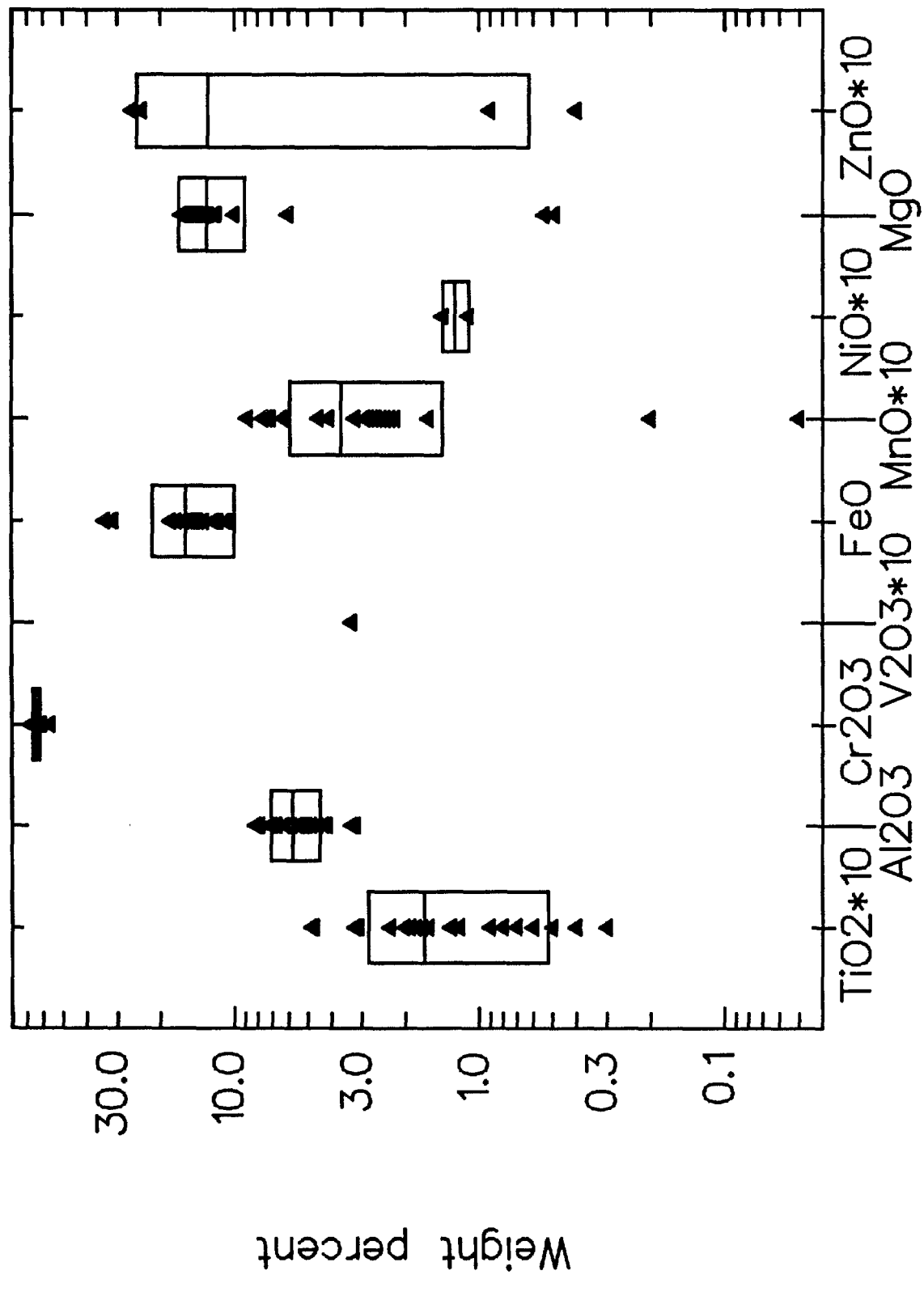
(13) Define pen for box

Option [1-13] (Exit):

Options 1-8 are similar to the options available for histogram plots. Option 9 is used to specify box size (0-5 standard deviations above and below the mean; default is 1.0). Option 10 enables the boxes to be omitted if desired, with option 11 the sample points inside boxes may be omitted, option 12 defines linear or log axes, and option 13 offers a choice of pen colours for the box.

The default Box-whisker Plot Definition File (BOXWHISK.DEF) comprises the major oxides. Suitable mineral reference files may be set up and expressions as well as concentrations incorporated as required. An example of the box-whisker plot to show compositional variation amongst chrome spinel inclusions in diamond is shown in Figure 5.

FIG. 5. BOX–WHISKER PLOT OF CHROMITES IN DIAMOND



## 6.17 PRINT STRUCTURAL FORMULAE REPORT

This option generates on file MDA.PRN a table of analyses and atomic proportions calculated using the number of oxygens and cations stored in the GDA data file. Ferric iron will only be calculated if non-zero values are held in both the cations and oxygens fields. The sample number, analysis number and mineral description fields are printed at the bottom of the table. An example is given in Table 2. The file MDA.PRN may be modified using a text editor prior to printing.

TABLE 2. EXAMPLE OF STRUCTURAL FORMULAE REPORT

STRUCTURAL FORMULAE - crnod.GDA

| | A | B | C | D | E |
|---|---|---|---|---|---|
| MgO | 12.82 | 15.42 | 14.84 | 14.70 | 14.72 |
| Al2O3 | 7.88 | 14.02 | 14.27 | 13.60 | 10.40 |
| SiO2 | .06 | <.02 | .03 | .03 | <.02 |
| CaO | <.02 | <.02 | <.02 | <.02 | <.02 |
| TiO2 | .10 | .11 | .20 | .21 | 1.73 |
| V2O3 | .17 | .00 | .30 | .28 | .23 |
| Cr2O3 | 64.68 | 57.49 | 57.59 | 57.63 | 57.53 |
| MnO | .16 | .12 | .12 | .09 | .14 |
| Fe2O3 | .54 | 2.84 | 1.05 | 1.56 | 3.00 |
| FeO | 13.60 | 10.80 | 11.61 | 11.62 | 12.46 |
| NiO | .07 | .13 | .10 | .14 | .19 |
| ZnO | .11 | .00 | .06 | .07 | .09 |
| Total | 100.18 | 100.93 | 100.17 | 99.94 | 100.49 |

Atomic Proportions.

| | | | | | |
|---|---|---|---|---|---|
| Ox | 4.0000 | 4.0000 | 4.0000 | 4.0000 | 4.0000 |
| Mg | .6241 | .7151 | .6940 | .6915 | .6989 |
| Al | .3033 | .5141 | .5277 | .5059 | .3904 |
| Si | .0020 | | .0009 | .0009 | |
| Ti | .0025 | .0026 | .0047 | .0050 | .0414 |
| V | .0045 | | .0075 | .0071 | .0059 |
| Cr | 1.6702 | 1.4142 | 1.4287 | 1.4381 | 1.4488 |
| Mn | .0044 | .0032 | .0032 | .0024 | .0038 |
| Fe+++ | .0132 | .0666 | .0248 | .0371 | .0720 |
| Fe++ | .3714 | .2811 | .3045 | .3068 | .3318 |
| Ni | .0018 | .0033 | .0025 | .0036 | .0049 |
| Zn | .0027 | | .0014 | .0016 | .0021 |
| Total | 3.0000 | 3.0000 | 3.0000 | 3.0000 | 3.0000 |

A: AR2/1 = AVERAGE 8 CHROMITE CORES
B: N38/1 = CHROMITE CORE
C: N41/1 = AVERAGE 8 CHROMITE CORES
D: N45/1 = AVERAGE 14 CHROMITE CORES
E: N45/2 = CHROMITE RIM

## 6.18 PRINT PYROXENES REPORT

This option generates, as a print file (MDA.PRN), a report of pyroxene analyses including structural formulae calculated on the basis of 4 cations per 6 oxygens. Site occupancy following the method of Wood and Banno (1973), atomic ratios (Ca/(Ca+Mg+Fe), etc.), and percent end member molecules. The pyroxene structure is examined for conformity to the ideal pyroxene formula and the program gives warnings if the number of oxygens in the formula sums to less than 6 or if any of the following rejection criteria apply:

- Si>2.02 or<1.98
- ACF2T - Ti + Mg + $Fe^{2+}$ + $Fe^{3+}$ + Mn + Ni <0.98 , where ACF2T = $Al^{M1}$ + Cr + $Fe^{3+}$ + 2Ti
- Sum of M2 cations <0.98 or> 1.02
- ACF2T - Ca - Na - K - $Al^{iv}$ >0.030
- Na >ACF2T

The percentage of pyroxene end-member components are calculated in the order $NaCrSi_2O_6$ (ureyite), $CaCr_2SiO_6$ (Ca-Cr-tschermaks), $NaAlSi_2O_6$ (jadeite), $NaFe^{3+}Si_2O_6$ (acmite), $CaTiAl_2O_6$ (Ca-Ti-tschermaks), $CaAl_2SiO_6$ (Ca-tschermaks), $CaFe^{3+}{}_2SiO_6$ (Ca-ferritschermaks), $CaSiO_3$ (wollastonite), $MgSiO_3$ (enstatite) and $FeSiO_3$ (ferrosilite) following a modified version of the method suggested by Cawthorn and Collerson (1974). The remaining unassigned cations are listed. For good quality analyses the percentage of unassigned cations should be less than 1%. The print file MDA.PRN may be printed direct or modified by word processor.

An example of the pyroxene report is given in Table 3.

**TABLE 3. EXAMPLE OF PYROXENE REPORT**

E9/8/1 Cpx

| oxides: | analysis: | ferric: | | cations: | | site occupancy: | | |
|---|---|---|---|---|---|---|---|---|
| SiO2 | 54.69 | 54.69 | Si | 1.965 | 1.963 | Al/2. | .193 | .192 |
| TiO2 | .68 | .68 | Ti | .018 | .018 | Al(T) | .035 | .037 |
| Al2O3 | 9.10 | 9.10 | Al | .385 | .385 | Al(M1) | .350 | .348 |
| Cr2O3 | .05 | .05 | Cr | .001 | .001 | Mg(M1) | .459 | .459 |
| Fe2O3 | .00 | .46 | Fe3+ | .000 | .012 | (ACF2T) | .388 | .398 |
| FeO | 6.30 | 5.89 | Fe2+ | .189 | .177 | T(tot) | 2.000 | 2.000 |
| MnO | .12 | .12 | Mn | .004 | .004 | M1(tot) | 1.000 | 1.000 |
| NiO | .00 | .00 | Ni | .000 | .000 | M2(tot) | 1.004 | 1.000 |
| MgO | 9.44 | 9.44 | Mg | .506 | .505 | ln(a)EN | -3.680 | -3.644 |
| CaO | 14.93 | 14.93 | Ca | .575 | .574 | mg# | 72.8 | 74.1 |
| Na2O | 4.85 | 4.85 | Na | .338 | .337 | | | |
| K2O | .51 | .51 | K | .023 | .023 | | | |
| Total | 100.67 | 100.72 | Sum | 4.004 | 4.000 | | | |

atomic ratios: Ca* 45.3 Mg* 39.8 Fe* 14.9

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| no ferric: | WO" | 44.7 | EN" | 40.2 | FS" | 15.1 | ---accepted 0 warning(s) |
| ferric: | WO" | 44.7 | EN" | 40.9 | FS" | 14.3 | ---accepted 0 warning(s) |

Molecular Percent End-members

| | | | |
|---|---|---|---|
| NaCrSi2O6 | (Ureyite) | Ur | .14 |
| CaCr2SiO6 | (Ca-Cr-tschermaks) | CaCrTs | .00 |
| NaAlSi2O6 | (Jadeite) | Jd | 36.04 |
| NaFe+++Si2O6 | (Acmite) | Ac | .00 |
| CaTiAl2O6 | (Ca-Ti-tschermak) | CaTiTs | 1.28 |
| CaAl2SiO6 | (Ca-tschermak) | CaTs | .00 |
| CaFe+++2SiO6 | (Ca-ferritschermak) | CaFeTs | .62 |
| CaSiO3 | (Wollastonite) | Wo | 27.83 |
| MgSiO3 | (Enstatite) | En | 25.32 |
| FeSiO3 | (Ferrosilite) | Fs | 8.76 |

Remaining Ti .006
Remaining Fe2+ .006
Percentage of unassigned cations is .28

## 6.19 PRINT AMPHIBOLES REPORT

This option allows calculation of amphibole end members in molecular percentages and the site allocations. It also provides an estimate of $Fe_2O_3$ content for microprobe analyses by normalisation of the the cations to either

- T + C = 13.0 exclusive of Ca, Na and K (recommended for the majority of amphiboles, especially calciferous varieties where Ca+Na>1.34)

or

- T + C + B = 15.0 exclusive of Na and K (recommended for Fe-Mg-Mn amphiboles).

The program calculates end members based on the 17 end-member amphiboles recognised by Hawthorne (1983), following a modified form of the method proposed by Currie (1991). The report is generated under MDA.PRN which can be edited and printed. The following end-member amphiboles are calculated:

Anthophyllite, gedrite, tremolite, hornblende, tschermakite, winchite, barroisite, $Na_2FM_3M_2Si_8O_{22}$ (riebeckite-glaucophane), Na-anthophyllite, Na-gedrite, edenite, $NaCa_2FM_4M_3Si_6O_{22}$ (hastingsite-pargasite), richterite, kataphorite, taramite, $Na_3FM_4MSi_8O_{22}$ (arfvedsonite-eckermannite), nyboite and kaersutite.

The amphibole structure is examined for conformity to the ideal amphibole structure and rejects analyses which violate the following conditions:

- Si + Al <8.00
- Si >8.00
- M1 cations >5.00, i.e., Cr + $Al^{vi}$+$Fe^{3+}$M1 + Ti >5.00
- Ca >2.00
- M4 site cation deficient
- Ca required in A-site
- A-site cations >1.00.

An example printout is given in Table 4.

**TABLE 4. EXAMPLE OF AMPHIBOLE REPORT**

AMPHIBOLES REPORT - wandamph.GDA

WANDAGEE/31475 AMPHIBOLE 3 GEN 256

| oxides | all FeO: | ferric: | | cations: | | Site allocation: | | |
|---|---|---|---|---|---|---|---|---|
| SiO2 | 41.62 | 41.62 | Si | 6.188 | 6.077 | Si | 6.188 | 6.077 |
| TiO2 | .74 | .74 | Ti | .083 | .081 | Al4 | 1.812 | 1.923 |
| Al2O3 | 13.92 | 13.92 | Al | 2.440 | 2.396 | Fe3 | .000 | .000 |
| Cr2O3 | .05 | .05 | Cr | .006 | .005 | | 8.000 | 8.000 |
| Fe2O3 | .00 | 7.53 | Fe3+ | .000 | .827 | Al6 | .629 | .473 |
| FeO | 14.23 | 7.46 | Fe2+ | 1.770 | .911 | Ti | .083 | .081 |
| MnO | .38 | .38 | Mn | .048 | .047 | Cr | .006 | .005 |
| NiO | .00 | .00 | Ni | .000 | .000 | Fe3 | .000 | .827 |
| ZnO | .00 | .00 | Zn | .000 | .000 | Fe-Mg | 4.283 | 3.613 |
| MgO | 12.19 | 12.19 | Mg | 2.703 | 2.654 | | 5.000 | 5.000 |
| CaO | 9.95 | 9.95 | Ca | 1.586 | 1.557 | Fe-Mg | .238 | .000 |
| Na2O | 3.84 | 3.84 | Na | 1.107 | 1.087 | Ca | 1.586 | 1.557 |
| K2O | 1.35 | 1.35 | K | .257 | .252 | Na | .176 | .443 |
| Total | 98.28 | 99.04 | Sum | 16.188 | 15.897 | | 2.000 | 2.000 |
| | | | | | | Na | .931 | .645 |
| | | | | | | K | .257 | .252 |
| | | | | | | | 1.188 | .897 |
| | | | | | | Total | 16.188 | 15.897 |

| | | | | | |
|---|---|---|---|---|---|
| Mg# | 60.4 | 74.5 | all FeO analysis: | ***rejected | 1 error(s) |
| Fe3# | .0 | 47.6 | ferric analysis: | ---accepted | 0 error(s) |
| Ca" | 26.2 | 30.4 | | | |
| Mg" | 44.6 | 51.8 | | | |
| Fe2" | 29.2 | 17.8 | | | |

End-members (Mol fraction)

| | | | | | |
|---|---|---|---|---|---|
| Fe-Mg amphibole | .000 | | | | |
| Ca-Na amphibole | 1.000 | | | | |
| A-site vacant | | | | | |
| Hornblende | .0019 | ferri- | .0012 | alumino- | .0007 |
| Tschermakite | .0556 | ferri- | .0353 | alumino- | .0202 |
| Barroisite | .0456 | ferri- | .0290 | alumino- | .0166 |
| A-site full | | | | | |
| Edenite | .0386 | ferri- | .0245 | alumino- | .0140 |
| NaCa2FM4MSi6Al2 | .3802 | Hastingsite | .2418 | Pargasite | .1384 |
| Kataphorite | .0306 | ferri- | .0195 | alumino- | .0111 |
| Taramite | .3663 | ferri- | .2330 | alumino- | .1333 |
| Kaersutite | .0812 | ferri- | .0516 | alumino- | .0295 |

## 6.20 PRINT AMPHIBOLE CLASSIFICATION REPORT

This option employs the program AMPHTAB (Rock, 1987) to calculate amphibole formula units and classify and name amphiboles according to the IMA (1978) scheme.

Options are available for calculation of $Fe^{3+}$ and for inclusion and treatment of $H_2O$, $CO_2$ and $P_2O_5$ contents. An example of output is given in Table 5 and full details are given by Rock (1987).

**TABLE 5. EXAMPLE OF AMPHIBOLE CLASSIFICATION REPORT**

```
Classify amphiboles using IMA(1978) scheme [Mineral.Mag.42,533-63]

 GDA file: wandamph.GDA
```

| | 1 | 2 | 3 |
|---|---|---|---|
| SiO2 | 40.73 | 41.35 | 41.62 |
| TiO2 | .67 | .37 | .74 |
| Al2O3 | 16.33 | 15.20 | 13.92 |
| Cr2O3 | .03 | .10 | .05 |
| Fe2O3 | .00 | .00 | .00 |
| FeO | 12.79 | 12.28 | 14.23 |
| MnO | .23 | .27 | .38 |
| MgO | 11.28 | 12.51 | 12.19 |
| CaO | 10.93 | 10.00 | 9.95 |
| Na2O | 3.58 | 4.02 | 3.84 |
| K2O | .86 | 1.30 | 1.35 |
| TOTAL | 97.43 | 97.41 | 98.37 |
| CATIONS PER FORMULA UNIT | | | |
| O= | 23.0 | 23.0 | 23.0 |
| Si | 6.002 | 6.055 | 6.077 |
| Al | 2.837 | 2.623 | 2.396 |
| Fe3+ | .369 | .650 | .827 |
| Fe2+ | 1.207 | .853 | .911 |
| Mg | 2.478 | 2.731 | 2.655 |
| Ca | 1.727 | 1.569 | 1.557 |
| Na | 1.022 | 1.141 | 1.087 |
| K | .162 | .244 | .252 |
| Ti | .074 | .041 | .081 |
| Mn | .029 | .034 | .047 |
| Cr | .003 | .012 | .005 |
| TOTAL | 15.911 | 15.953 | 15.897 |
| CHECK ON OXYGEN(+Cl,F) EQUIVALENCE OF ABOVE CATIONS | | | |
| O= | 23.00 | 23.00 | 23.00 |
| IMA(1978) CLASSIFICATION PARAMETERS | | | |
| CaNa | 2.000 | 2.000 | 2.000 |
| NaB | .273 | .431 | .443 |
| NaKA | .911 | .953 | .897 |
| AlVI | .839 | .678 | .473 |
| MgFe | .672 | .762 | .745 |

TABLE 5. CONTINUED

GENERAL NOTES FOR THE ABOVE TABLE:
P2O5 (where quoted) has been treated as zero in calculation of formula unit. Results have not been checked or adjusted for low water/high cation totals. Fe has been reallocated wherever possible between Fe3 and Fe2, where only total Fe is quoted.

IMA(1978)Names for the above Table:

Analysis: WANDAGEE/31473 Number: 1
Sum of cations S2 brought to 13.0 by redistribution of total Fe between Fe2 & Fe3
SODIAN
FERROAN PARGASITE

Analysis: WANDAGEE/31474 Number: 2
Sum of cations S2 brought to 13.0 by redistribution of total Fe between Fe2 & Fe3
SODIAN
PARGASITE

Analysis: WANDAGEE/31475 Number: 3
Sum of cations S2 brought to 13.0 by redistribution of total Fe between Fe2 & Fe3
POTASSIAN
SODIAN
MAGNESIO-HASTINGSITE

## 6.21 PRINT SPINELS REPORT

Option 6.21 generates on the MDA print file (MDA.PRN) a report of spinel compositions with ferric contents calculated assuming 3 cations for 4 oxygens. Spinel end-numbers are calculated in the order $ZnAl_2O_4$, $MgAl_2O_4$, $Mg_2TiO4$, $Mn_2TiO_4$, $Fe_2TiO4$, $MgCr_2O_4$, , $MnCr_2O_4$, $FeCr_2O_4$, and $Fe_3O_4$ following a modified version of the method of Mitchell and Clarke (1976). An example of the output is given in Table 6.

**TABLE 6. EXAMPLE OF SPINEL REPORT**

SPINELS REPORT - splherz.GDA

| Analysis 75210425A2/1 | Wt % | O= 4.0 | SPINEL ppm |
|---|---|---|---|
| MgO | 19.03 | .7737 | 114771 |
| Al2O3 | 43.33 | 1.3930 | 229324 |
| SiO2 | .07 | .0019 | 327 |
| CaO | <.02 | | <143 |
| TiO2 | .47 | .0096 | 2818 |
| V2O3 | .08 | .0017 | 544 |
| Cr2O3 | 24.17 | .5213 | 165372 |
| MnO | .07 | .0016 | 542 |
| Fe2O3 | 2.97 | .0609 | 20748 |
| FeO | 9.96 | .2272 | 77426 |
| NiO | .30 | .0066 | 2358 |
| ZnO | .12 | .0024 | 964 |
| Total | 100.57 | 3.0000 | |

| Reduced | | Oxidised | |
|---|---|---|---|
| 100Mg/(Mg+Fe) | 72.866 | 100Mg/(Mg+Fe2+) | 77.299 |
| 100Al/(Al+Cr+2Ti) | 72.044 | 100Al/(Al+Cr+Fe3+) | 70.526 |
| 100Cr/(Al+Cr+2Ti) | 26.959 | 100Cr/(Al+Cr+Fe3+) | 26.391 |
| 200Ti/(Al+Cr+2Ti) | .997 | 100Fe3+/(Al+Cr+Fe3+) | 3.083 |
| 100Cr/(Cr+Al) | 27.231 | 100Cr/(Cr+Al) | 27.231 |

| End members | |
|---|---|
| ZnAl2O4 | .242 |
| MgAl2O4 | 69.408 |
| FeAl2O4 | .000 |
| MnAl2O4 | .000 |
| Mg2TiO4 | 1.155 |
| Mn2TiO4 | .000 |
| Fe2TiO4 | .000 |
| MgCr2O4 | 6.311 |
| FeCr2O4 | 19.678 |
| MnCr2O4 | .162 |
| Fe3O4 | 3.044 |

## 6.22 PRINT GARNET REPORT

This option generates a report on garnet analyses as a print file (MDA.PRN), which may be output direct to a printer or first modified by word processor. The program allocates cations to sites, calculates ferric iron assuming 8 cations for 12 oxygens, and calculates garnet end-member components in the order $NaCa_2AlSi_4O_{12}$ (Majorite), $Y_3Al_2Al_3O_{12}$ (Yttrogarnet), $Mn_3V_2Si_3O_{12}$ (Yamatoite), $Ca_3V_2Si_3O_{12}$ (Goldmanite), $Ca_3Zr_2Al_2SiO_{12}$ (Kimzeyite), $Ca_3Zr_2Fe^{3+}SiO_{12}$ (Ferric-Kimzeyite), $Ca_3Cr_2Si_3O_{12}$ (Uvarovite), $Mg_3Cr_2Si_3O_{12}$ (Knorringite), $Ca_3Ti_2Fe^{3+}TiO_{12}$ (Schorlomite), $Ca_3Fe^{3+}{}_2Si_3O_{12}$ (Andradite), $Mg_3Al_2Si_3O_{12}$ (Pyrope), $Mn_3Al_2Si_3O_{12}$ (Spessartine), $Ca_3Al_2Si_3O_{12}$ (Grossular), $Fe^{2+}Al_2Si_3O_{12}$ (Almandine), $Mg_3Fe^{3+}{}_2Si_3O_{12}$ (Koharite), $Fe^{2+}Fe^{3+}{}_2Si_3O_{12}$ (Skiagite), $Mn_3Fe^{3+}{}_2Si_3O_{12}$ (Calderite), and $Mn^{2+}{}_3Mn^{3+}{}_2Si_3O_{12}$ (Blythite), following a modified form of the method of Rickwood (1968). Remaining cations should be less than 1% for a good analysis. The common garnets are classified and named according to the Dawson and Stephens (1975) classification scheme. An example of output is given in Table 7.

**TABLE 7. EXAMPLE OF GARNET REPORT**

GARNET REPORT - akconga.GDA

ARGYLE/31382 CONCENTRATE LDC 0-4-12

| oxides: | analysis: | ferric: | cations: | | | site occupancy: | | |
|---|---|---|---|---|---|---|---|---|
| P2O5 | .04 | .04 | P | .002 | .002 | SiTET | 2.984 | 2.973 |
| ZrO2 | .00 | .00 | Zr | .000 | .000 | AlTET | .016 | .027 |
| SiO2 | 42.06 | 42.06 | Si | 2.981 | 2.970 | TiTET | .000 | .000 |
| TiO2 | .70 | .70 | Ti | .037 | .037 | Fe3+TET | .000 | .000 |
| Al2O3 | 21.59 | 21.59 | Al | 1.804 | 1.797 | SUM | 3.000 | 3.000 |
| Cr2O3 | 1.81 | 1.81 | Cr | .101 | .101 | SiY | .000 | .000 |
| V2O3 | .00 | .00 | V | .000 | .000 | AlY | 1.787 | 1.770 |
| Y2O3 | .00 | .00 | Y | .000 | .000 | Fe3Y | .000 | .088 |
| Fe2O3 | .00 | 1.66 | Fe3+ | .000 | .088 | TiY | .037 | .037 |
| FeO | 7.40 | 5.91 | Fe2+ | .439 | .349 | Y-Site | 1.926 | 1.996 |
| MnO | .24 | .24 | Mn | .014 | .014 | X-Site | 3.104 | 3.004 |
| NiO | .00 | .00 | Ni | .000 | .000 | | | |
| MgO | 21.93 | 21.93 | Mg | 2.317 | 2.309 | | | |
| CaO | 4.28 | 4.28 | Ca | .325 | .324 | | | |
| Na2O | .06 | .06 | Na | .008 | .008 | | | |
| Total | 100.11 | 100.28 | Sum | 8.029 | 8.000 | | | |

atomic ratios: Ca* 10.5 Mg* 75.2 Fe* 14.2

100Mg/(Mg+Fe2+): 86.9

100Mg/(Mg+Fe): 84.1

Molecular Percent End-members

| | | | |
|---|---|---|---|
| NaCa2AlSi4O12 | (Majorite) | Maj | .82 |
| Y3Al2Al3O12 | (Yttrogarnet) | Yt | .00 |
| Mn3V2Si3O12 | (Yamatoite) | Ya | .00 |
| Ca3V2Si3O12 | (Goldmanite) | Gold | .00 |
| Ca3Zr2Al2SiO12 | (Kimzeyite) | Kimz | .00 |
| Ca3Zr2Fe3+2SiO12 | (Ferric-Kimzeyit | Fe-Kimz | .00 |
| Ca3Cr2Si3O12 | (Uvarovite) | Uvar | 5.07 |
| Mg3Cr2Si3O12 | (Knorringite) | Knor | .00 |
| Ca3Ti2Fe3+2TiO12 | (Schorlomite) | Sch | 1.24 |
| Ca3Fe3+2Si3O12 | (Andradite) | And | 3.18 |
| Mg3Al2Si3O12 | (Pyrope) | Py | 77.17 |
| Mn3Al2Si3O12 | (Spessartine) | Sp | .48 |
| Ca3Al2Si3O12 | (Grossular) | Gr | .79 |
| Fe2+Al2Si3O12 | (Almandine) | Alm | 11.25 |
| Mg3Fe3+2Si3O12 | (Koharite) | Koh | .00 |
| Fe2+3Fe3+2Si3O12 | (Skiagite) | Ski | .00 |
| Mn3Fe3+2Si3O12 | (Calderite) | Cal | .00 |
| Mn2+3Mn3+2Si3O12 | (Blythite) | Bly | .00 |

Remaining Si .010
Remaining Fe2+ .012
Percentage of unassigned cations is .28

Dawson & Stephens - group no 1 Titanian pyrope

# 7 VECTOR

Plot (i.e., graphics) files generated in BMRMDA (generally with names between GDA1.VEC and GDA99.VEC) using the SciPlot Graphics package can be output to various devices, either directly, or,for some plot file types, using the VECTOR program. A number of different graphics file types is available, and the one required must be specified when generating plot files in BMRMDA (see above). However, plotter and printer metafiles may be output to either device (although the size may need changing), or displayed on screen. Examples of mineral plots generated in BMRMDA and output to laser printer from HPGL files are given in Figures 1 - 8.

The Postscript file is an ASCII file that may be edited or sent directly to any Postscript printer. The Encapsulated Postscript file (EPS) and the Computer Graphics Metafile (CGM), an ANSI standard format file, are files that should not be edited for they contain binary information. EPS and CGM files can be imported directly into word processors or other graphical products. The HP pen plotter file (HPGL) is an ASCII file that can be edited and imported into word processors or other graphical products. The WordPerfect file (WPG) is a binary file in WordPerfect's internal graphics format. WPG files are directly importable into the WordPerfect word processor. The SciPlot Graphics metafile is a file in SciPlot's own internal format and is used solely as input to the VECTOR program. This file is a binary file in very compact format. It contains the stream of vectors which represent the figures, characters, etc. generated during the execution of the application program. VECTOR processes this graphic file and arranges raw vectors in the direction of paper motion order before display on dot matrix printers and laserjet printers. For Apple LaserWriters, HP pen plotters, and other graphics devices that support vector drawing commands directly, ordering is not required and VECTOR immediately displays the vectors. VECTOR's function is to provide a utility to register SciPlot's output on plotting devices (dot matrix and laserjet printers) which cannot be supported directly without requiring significant system resources. VECTOR also provides interactive preview of graphics files on the screen or batch processing at some other time.

There is no paper positioning done by VECTOR. Therefore, the user must position the paper before executing the VECTOR program. This is done purposefully to allow plots to be manually positioned. It is possible to imbed plots in full text with a careful alignment of the paper.

The HP Pen Plotter, the HP LaserJet, and the Apple LaserWriter are all supported by VECTOR to register the graphics files produced by SciPlot.

## 7.1 VECTOR PROGRAM

VECTOR has two modes of operation, an interactive mode and a batch mode. The batch mode processes command strings from a disk file, which contains a list of plot file names (e.g. GDA1.VEC, GDA2.VEC etc.). The user can include the command file name, with the VECTOR command (e.g. VECTOR command.fil). Alternatively, the user can wait until VECTOR issues a prompt for the type of processing required. The interactive mode is used to process single plot files, as generated in BMRMDA.

The VECTOR.CFG configuration file contains a list of commands that define VECTOR processing parameters. Each time VECTOR is executed it reads and interprets this file. If the VECTOR.CFG file cannot be located, VECTOR will interact with the user from the terminal to set up these parameters.

An example of a VECTOR.CFG file is as follows:

```
FILE=CONS
DEVICE=DOT
PORT=LPT1
HAND=SOFT
MODE=195
HRES=LOW
VRES=LOW
ANGL=0.0
XSCL=1.0
YSCL=1.0
XOFS=0.0
YOFS=0.0
WAIT=ON
PINS=9
INIT=ON
```

To run the program, type VECTOR. The parameters contained in VECTOR.CFG will be used to define the output device, format of the plot, etc. If these need to be changed, type VECTOR /U.

This update option overrides all the parameters specified in the VECTOR.CFG file. An interactive dialogue is initiated to obtain a new set of parameters for VECTOR. The user is given the opportunity at the end of the dialogue to update the current VECTOR.CFG file with these new parameters. If no VECTOR.CFG file exists, typing VECTOR alone will initiate this dialogue.

The following questions must be answered (defaults, as stored on VECTOR.CFG file, in square brackets, and valid responses are shown):

1. Process File [CONS]:
   [d:\path\filename.ext ]
   [CONS = Console keyboard ]

   [d:\path\filename.ext] - Process file which contains file names of graphics files to be processed in batch mode. These files will be processed one at a time and plotted on the designated printer, plotter, or monitor screen. As a default, the VECTOR.CFG file will be searched for a process file name. When a file name is specified on the VECTOR command line, the process file name given in VECTOR.CFG file is totally ignored and replaced by this new file name.

CONS - Enter graphic file names from console (keyboard).

2. Output Device [DOT ]:
   [DOT = Dot Matrix Printer ]
   [PEN =HP Pen Plotter ]

[JET =HP Laser Jet Printer ]
[WRITER = Apple LaserWriter Printer ]
[CGA = CGA Graphics Screen ]
[EGA = EGA Graphics Screen ]
[VGA = VGA Graphics Screen ]
[HGA = Hercules Graphics Screen ]

3. Vertical Plot Resolution [LOW ]:
   [LOW = Low Resolution ]
   [HIGH =High Resolution ]

   For dot matrix type graphics printers, four basic resolutions are provided by VECTOR depending on the type of printer attached. A low resolution mode is supported to quickly review the plot with very limited definition. This mode is useful for quick turn-around. The high resolution mode takes much more time because of hardware constraints, but gives very satisfactory results.

4. Horizontal Plot Resolution [LOW ]:
   [LOW = Low Resolution ]
   [HIGH = High Resolution ]

5. Dot Matrix Pin Type [9 ]:
   [9 = EPSON (MX-80,FX-80,FX-85) ]
   [24 = EPSON (LQ-800/1000) ]

6. Output I/O Port [LPT1]:
   [COM1 = COM1 Serial Port ]
   [COM2 = COM2 Serial Port ]
   [LPT1 = LPT1 Parallel Port ]
   [LPT2 = LPT2 Parallel Port ]

7. Serial Port Handshake [SOFT]:
   [SOFT = Software - XON/XOFF ]
   [HARD = Hardware - DSR ]

8. Serial Port Modeset [195]:
   [xxx = Modeset code ]

   When the serial port is used for printer/plotter device, the following commands are valid:

   HAND = SOFT - Software Handshake (XON/XOFF)

   = HARD - Hardware flow control on DSR line

   MODE = 195 - Serial Port Mode Set Code, specified in decimal format. 195 = (9600 baud, no parity, 1 stop bit, 8 bit characters)

   - Mode Set Code Description - [bits]

| 7 6 5 | 4 3 | 2 | 1 0 |
|---|---|---|---|
| -Baud Rate- | -Parity- | -Stop Bits- | -Char Length- |
| 000 - 110 | 00 - None | 0 - 1 | 10 - 7 Bits |
| 001 - 300 | 01 - Odd | 1 - 2 | 11 - 8 Bits |
| 010 - 600 | 11 - Even | | |
| 011 - 1200 | | | |
| 100 - 2400 | | | |
| 101 - 4800 | | | |
| 110 - 9600 | | | |
| 111 - 19200 | | | |

9. HP Handshake Initialisation [ON ]:
   [ON = Send before plotting]
   [OFF = None required ]

   When an HP Pen plotter is used, the following plotter initialisation command is valid.

   INIT = ON - Send handshake init sequence before plotting

   = OFF - No handshake init sequence required

10. Rotation Angle(deg) [ .00]:
    [xxx.xx = Angle(deg)]

11. X-Axis Scale [ 1.00]:
    [ x.xx = Scale factor]

12. Y-Axis Scale [ 1.00]:
    [ x.xx = Scale factor]

13. X-Axis Offset (inches) [ .00]:
    [ xx.xx = Offset (inches)]

14. Y-Axis Offset (inches) [ .00]:
    [ xx.xx = Offset (inches)]

15. Crt Wait Flag [ON]:
    [ON = Wait between frames ]
    [OFF = No wait between frames ]

    For batch processing mode only

16. Update VECTOR.CFG file [NO]:
    [NO = No update]
    [YES = Update ]

    This allows the vector configuration file to be updated with the new parameters, if desired.

17. Graphics File [null]:
    [d:\path\filename.ext]

The name of the file to be processed is given. If none, program is terminated.

Note that not all the above questions will be asked in every case; it will depend on the output device chosen.

Options 10 - 14 allow plots to be formatted on the page. For example, plots with different X-axis variables may be stacked by specifying the appropriate X and Y-axis offsets. Similarly, a legend may be positioned under the relevant plot. Plot size may be changed by specifying X and Y-axis scale factors. Rotation allows plots to be re-orientated on the page, but note that an X-axis offset will also be necessary, or the plot is rotated off the page!

# 8 PRINT A TABLE OF MINERAL ANALYSES (TABMIN)

Tables of mineral analyses, including cation proportions in the structural formula, can be generated by selecting 14 on the GDA-MDA menu or by directly calling the program TABMIN. The tables generated have a different format from those generated by option 17 of the BMRMDA program (print structural formulae reports). TABMIN output allows reporting of trace elements and arithmetic derivatives for the analyses, including weight and atomic ratios, such as $Ca/(Ca+Mg+Fe^{2+})$,etc. The print file generated – TABMIN.PRN – may be edited/enhanced to camera-ready format using a wordprocessor. The program is run by entering TABMIN which generates the following menu:

Print oxides GDA file [Y/N = metals] (Y):

Geochemical file name [? = LIST] (CURRENT.GDA ): **FILENAME**

Report/statistics definition file [? = LIST] (OXIDE.MTB ):

Mineral definitions file [? = LIST] (OXIDE.DEF):

Print trace elements [Y/N] (N)?

Print Geochemical Data

(1) Generate report on print file TABMIN.PRN

(2) Display report on screen

(3) Display structural formula for single analysis

(4) Select major elements

(5) Select trace elements (element values in parts per million)

(6) Select structural formula components

(7) Specify descriptive fields

(9) Select groups to be printed or displayed

(10) Specify range of analyses

(11) Specify group titles

(13) Specify number of analyses per printer page

(14) Specify number of lines on printer page

(16) Print values for typed in expressions (derived from structural formulae)

(18) Include page header

(19) Change GDA file

Q = Quit

Option [1-19,Q]:

These options allow full selection of descriptive fields, analytical data and derived values (option 16).

Report definition file OXIDE.MTB is used for silicate and oxide analyses, whereas METAL.MTB is used for metals and sulphides. These define the names of major and trace elements for output. For printing of trace elements, oxide or element weight percentages are converted to parts per million, using (where applicable) oxide factors stored in OXIDE.DEF

An example of the output from TABMIN is shown in Table 8.

**TABLE 8. EXAMPLE OF OUTPUT FROM TABMIN**

DIAMONDIFEROUS XENOLITHS

| Sample number | N44 | N14 | N40 | N27 |
|---|---|---|---|---|
| Analysis number | 1 | 2 | 3 | 4 |
| Mineral name | OLIVINE | OLIVINE | OLIVINE | OLIVINE |
| Description | P1 OLIVINE | P1 OLIVINE | P1 OLIVINE | P1 OLIVINE |
| SiO2 | 41.42 | 41.20 | 41.05 | 40.87 |
| Cr2O3 | .07 | .07 | .05 | .05 |
| FeO | 6.79 | 7.30 | 7.57 | 8.58 |
| MnO | .09 | .11 | .10 | .13 |
| NiO | .39 | .44 | .38 | .40 |
| MgO | 51.58 | 51.55 | 50.85 | 50.08 |
| CaO | .02 | .05 | .05 | .05 |
| Total | 100.36 | 100.72 | 100.05 | 100.16 |
| Trace elements in parts per million | | | | |
| Cr | 472 | 465 | 343 | 318 |
| Mn | 692 | 815 | 776 | 988 |
| Ni | 3064 | 3481 | 3015 | 3169 |
| Ca | 143 | 387 | 346 | 354 |
| Atomic proportions | | | | |
| Oxygens | 4.0 | 4.0 | 4.0 | 4.0 |
| Si | .999 | .993 | .997 | .996 |
| Cr | .001 | .001 | .001 | .001 |
| Fe2+ | .137 | .147 | .154 | .175 |
| Mn | .002 | .002 | .002 | .003 |
| Ni | .008 | .009 | .007 | .008 |
| Mg | 1.854 | 1.852 | 1.840 | 1.819 |
| Ca | .001 | .001 | .001 | .001 |
| Total | 3.001 | 3.006 | 3.003 | 3.003 |
| 100Mg/(Mg+Fe) | 93.12 | 92.64 | 92.29 | 91.23 |

# 9 STATS (STATISTICS PROGRAM)

The STATS program generates, on the print file STATS.PRN, various statistical functions including mean, standard deviation, minimum, maximum, and optional correlation matrix. A menu, shown below, enables selection of groups, elements and specification of format. The minerals report definition files OXIDE.RPT and METAL.RPT are employed to define output for oxides/silicates and metals/suphides, respectively They can be modified as required to include other fields (including trace elements). The program STATS is also used to generate a cluster analysis file for use in the cluster analysis program CLUSTA, details of which are given in section 10. Options 2-4, and 7-9 also apply in this case. The program is run by typing STATS or selecting option 6 from the GDA-MDA menu. 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; only expressions involving element or oxide concentrations as defined in the selected report defintion file may be used)

(9) Drop samples (anomalous samples may be deleted 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

Q = Quit

A typical printout is given in Table 9.

**TABLE 9. EXAMPLE OF OUTPUT FROM STATS PROGRAM**

GROUPS PROCESSED

PIPE M97 GARNETS
PIPE M89 GARNETS

MEANS AND STANDARD DEVIATIONS

| Element | Mean | Standard Deviation | Minimum | Maximum | Number of Items |
|---|---|---|---|---|---|
| P2O5 | .02 | .01 | .02 | .05 | 21 |
| SiO2 | 41.10 | .95 | 38.28 | 42.29 | 21 |
| TiO2 | .29 | .14 | .01 | .50 | 21 |
| Al2O3 | 18.89 | 2.46 | 12.57 | 22.50 | 21 |
| Cr2O3 | 5.91 | 3.08 | .01 | 13.31 | 21 |
| FeO | 8.17 | 4.60 | 6.71 | 28.23 | 21 |
| MnO | .35 | .13 | .24 | .89 | 21 |
| NiO | .02 | .01 | .02 | .04 | 21 |
| MgO | 19.64 | 3.02 | 7.40 | 22.12 | 21 |
| CaO | 6.10 | 1.11 | 3.72 | 9.29 | 21 |
| Na2O | .04 | .02 | .01 | .09 | 21 |
| mg | 80.94 | 11.30 | 31.85 | 84.83 | 21 |

CORRELATION MATRIX

| | P2O5 | SiO2 | TiO2 | Al2O3 | Cr2O3 | FeO |
|---|---|---|---|---|---|---|
| P2O5 | 1.00 | | | | | |
| SiO2 | -.21 | 1.00 | | | | |
| TiO2 | -.24 | .42 | 1.00 | | | |
| Al2O3 | -.41 | .38 | .13 | 1.00 | | |
| Cr2O3 | .43 | -.25 | -.12 | -.98 | 1.00 | |
| FeO | -.15 | -.69 | -.45 | .30 | -.43 | 1.00 |
| MnO | -.17 | -.74 | -.52 | .25 | -.36 | .95 |
| NiO | -.19 | -.01 | .12 | .00 | .00 | -.06 |
| MgO | .02 | .88 | .55 | .02 | .11 | -.93 |
| CaO | .38 | -.18 | -.15 | -.91 | .94 | -.48 |
| Na2O | .03 | -.32 | .40 | -.24 | .21 | -.08 |
| mg | .12 | .74 | .48 | -.24 | .38 | -1.00 |

CORRELATION MATRIX

| | MnO | NiO | MgO | CaO | Na2O | mg |
|---|---|---|---|---|---|---|
| FeO | | | | | | |
| MnO | 1.00 | | | | | |
| NiO | -.02 | 1.00 | | | | |
| MgO | -.94 | .08 | 1.00 | | | |
| CaO | -.37 | .01 | .14 | 1.00 | | |
| Na2O | .01 | .28 | -.02 | .19 | 1.00 | |
| mg | -.96 | .06 | .96 | .42 | .07 | 1.00 |

# 10 CLUSTA (CLUSTER ANALYSIS)

Option 7 of the main GDA-MDA menu provides a facility for cluster analysis. 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., measurements, 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).

It is important to note that any dataset for which a major proportion of samples have zero values should be omitted from the calculations, or the results may well be biased. In particular, if all *selected* samples have zero (i.e., no data) values for any dataset, or if all non-zero values are the same, an error will result when running the program. The offending dataset should be omitted and the cluster analysis file regenerated (in STATS). However, note that if all *assigned* samples have zero values, the dataset is automatically dropped out.

To run the program (which actually includes two parts, CLUSTA and BMRDEND), type CLUSTER or option 7 from the GDA-MDA starting menu.

The name of a cluster analysis cluster analysis file (normally of the form ????.CLU) must be given. This 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:

- Q-mode (default) or R-mode.
- The similarity measure-correlation coefficient (default) or proportional similarity coefficient.
- The linkage method - weighted-pair group method (default) or unweighted.
- Highest value of similarity (i.e., the upper limit of the Y-axis: 0-1, 1.0 by default).
- 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. Typically, 100 samples for 40 variables will take up to 15 minutes, depending on the PC. The input data,

transformed data matrix, cluster data and dendrogram details can be printed out from a file CLUSTA.PRN if required. Example printouts of Q-mode and R-mode cluster analysis for a suite of garnets from the Wandagee alkaline intrusives are given in Tables 10 and 11.

TABLE 10. EXAMPLE OF CLUSTER ANALYSIS (Q-MODE)

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

FROM STATS PROGRAM NUMBER OF SAMPLES = 21 NUMBER OF ELEMENTS = 7

CLUSTERING BY THE UNWEIGHTED PAIR-GROUP METHOD USING CORRELATION COEFFICIENT OF ASSOCIATION

PRINTOUT OF DATA MATRIX

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| WANDAGEE/31457 | .1500 | 18.0200 | 8.0000 | 7.0400 | .3100 | 19.7000 | 6.9100 |
| WANDAGEE/31458 | .4400 | 19.1800 | 5.4500 | 7.5400 | .3000 | 20.8700 | 5.5600 |
| WANDAGEE/31460 | .2000 | 18.0400 | 6.9900 | 6.7500 | .2600 | 20.9500 | 6.1700 |
| WANDAGEE/31461 | .2200 | 20.0300 | 4.9100 | 6.7100 | .3300 | 20.6100 | 5.9100 |
| WANDAGEE/31462 | .3600 | 20.0000 | 4.6000 | 7.2400 | .3800 | 20.2900 | 5.5600 |
| WANDAGEE/31463 | .1700 | 21.3900 | 3.5600 | 6.9200 | .3100 | 21.0800 | 5.4200 |
| WANDAGEE/31464 | .3900 | 19.3900 | 5.0700 | 7.0500 | .3300 | 20.7500 | 5.8800 |
| WANDAGEE/31465 | .4000 | 18.8800 | 5.3700 | 7.1000 | .2600 | 20.5600 | 5.9600 |
| WANDAGEE/31466 | .5000 | 20.9900 | 2.8200 | 7.3400 | .2400 | 22.1200 | 4.8000 |
| WANDAGEE/31467 | .4100 | 20.6500 | 3.5400 | 7.5800 | .3200 | 21.1700 | 5.3900 |
| WANDAGEE/31468 | .2400 | 22.5000 | 1.8900 | 7.0200 | .2700 | 22.0300 | 5.0600 |
| WANDAGEE/31476 | .1200 | 13.8500 | 11.9600 | 7.2200 | .3600 | 18.6800 | 7.6100 |
| WANDAGEE/31477 | .0900 | 12.5700 | 13.3100 | 7.5400 | .3300 | 17.1200 | 9.2900 |
| WANDAGEE/31478 | .4100 | 16.2600 | 8.7700 | 6.8500 | .2900 | 19.5500 | 6.8700 |
| WANDAGEE/31479 | .3800 | 18.2200 | 6.6800 | 7.2700 | .3800 | 19.0500 | 6.7200 |
| WANDAGEE/31480 | .3300 | 17.4600 | 8.0000 | 6.9800 | .2900 | 20.3200 | 5.8900 |
| WANDAGEE/31481 | .1900 | 20.0100 | 5.1300 | 7.0600 | .3600 | 20.2900 | 6.2100 |
| WANDAGEE/31482 | .4300 | 18.2600 | 6.9500 | 7.5600 | .3600 | 19.2200 | 6.8100 |
| WANDAGEE/31483 | .2100 | 20.2700 | 4.6100 | 7.4500 | .4000 | 20.2800 | 6.0500 |
| WANDAGEE/31484 | .4500 | 18.4200 | 6.5000 | 7.0700 | .2800 | 20.4000 | 6.2900 |
| WANDAGEE/31485 | .0100 | 22.2200 | .0100 | 28.2300 | .8900 | 7.4000 | 3.7200 |

TABLE 10 continued

VARIABLES TRANSFORMED TO PERCENT OF THEIR RANGE

PRINTOUT OF TRANSFORMED DATA MATRIX

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| WANDAGEE/31457 | .2857 | .5488 | .6008 | .0153 | .1077 | .8356 | .5727 |
| WANDAGEE/31458 | .8776 | .6657 | .4090 | .0386 | .0923 | .9151 | .3303 |
| WANDAGEE/31460 | .3878 | .5509 | .5248 | .0019 | .0308 | .9205 | .4399 |
| WANDAGEE/31461 | .4286 | .7513 | .3684 | .0000 | .1385 | .8974 | .3932 |
| WANDAGEE/31462 | .7143 | .7482 | .3451 | .0246 | .2154 | .8757 | .3303 |
| WANDAGEE/31463 | .3265 | .8882 | .2669 | .0098 | .1077 | .9293 | .3052 |
| WANDAGEE/31464 | .7755 | .6868 | .3805 | .0158 | .1385 | .9069 | .3878 |
| WANDAGEE/31465 | .7959 | .6354 | .4030 | .0181 | .0308 | .8940 | .4022 |
| WANDAGEE/31466 | 1.0000 | .8479 | .2113 | .0293 | .0000 | 1.0000 | .1939 |
| WANDAGEE/31467 | .8163 | .8137 | .2654 | .0404 | .1231 | .9355 | .2998 |
| WANDAGEE/31468 | .4694 | 1.0000 | .1414 | .0144 | .0462 | .9939 | .2406 |
| WANDAGEE/31476 | .2245 | .1289 | .8985 | .0237 | .1846 | .7663 | .6984 |
| WANDAGEE/31477 | .1633 | .0000 | 1.0000 | .0386 | .1385 | .6603 | 1.0000 |
| WANDAGEE/31478 | .8163 | .3716 | .6586 | .0065 | .0769 | .8254 | .5655 |
| WANDAGEE/31479 | .7551 | .5690 | .5015 | .0260 | .2154 | .7914 | .5386 |
| WANDAGEE/31480 | .6531 | .4924 | .6008 | .0125 | .0769 | .8777 | .3896 |
| WANDAGEE/31481 | .3673 | .7492 | .3850 | .0163 | .1846 | .8757 | .4470 |
| WANDAGEE/31482 | .8571 | .5730 | .5218 | .0395 | .1846 | .8030 | .5548 |
| WANDAGEE/31483 | .4082 | .7754 | .3459 | .0344 | .2462 | .8750 | .4183 |
| WANDAGEE/31484 | .8980 | .5891 | .4880 | .0167 | .0615 | .8832 | .4614 |
| WANDAGEE/31485 | .0000 | .9718 | .0000 | 1.0000 | 1.0000 | .0000 | .0000 |

**TABLE 10 continued**

FROM STATS PROGRAM

CLUSTERING BY THE UNWEIGHTED PAIR-GROUP METHOD

| SAMPLE NUMBERS | | LEVEL OF ASSOCIATION | CYCLE NUMBER |
|---|---|---|---|
| 1 | 3 | .9934 | 1 |
| 2 | 8 | .9984 | 1 |
| 6 | 11 | .9945 | 1 |
| 12 | 13 | .9879 | 1 |
| 15 | 18 | .9992 | 1 |
| 17 | 19 | .9989 | 1 |
| 2 | 7 | .9983 | 2 |
| 17 | 4 | .9983 | 2 |
| 2 | 20 | .9966 | 3 |
| 5 | 10 | .9971 | 3 |
| 2 | 5 | .9927 | 4 |
| 17 | 6 | .9865 | 4 |
| 14 | 16 | .9918 | 4 |
| 14 | 15 | .9908 | 5 |
| 2 | 9 | .9869 | 6 |
| 2 | 14 | .9799 | 7 |
| 17 | 1 | .9716 | 8 |
| 17 | 2 | .9635 | 9 |
| 17 | 12 | .8613 | 10 |
| 17 | 21 | .6489 | 11 |

ORDER OF SAMPLES FOR DENDROGRAM PLOT

| | |
|---|---|
| WANDAGEE/31481 | 17 |
| WANDAGEE/31483 | 19 |
| WANDAGEE/31461 | 4 |
| WANDAGEE/31463 | 6 |
| WANDAGEE/31468 | 11 |
| WANDAGEE/31457 | 1 |
| WANDAGEE/31460 | 3 |
| WANDAGEE/31458 | 2 |
| WANDAGEE/31465 | 8 |
| WANDAGEE/31464 | 7 |
| WANDAGEE/31484 | 20 |
| WANDAGEE/31462 | 5 |
| WANDAGEE/31467 | 10 |
| WANDAGEE/31466 | 9 |
| WANDAGEE/31478 | 14 |
| WANDAGEE/31480 | 16 |
| WANDAGEE/31479 | 15 |
| WANDAGEE/31482 | 18 |
| WANDAGEE/31476 | 12 |
| WANDAGEE/31477 | 13 |
| WANDAGEE/31485 | 21 |

FROM STATS PROGRAM

INFORMATION REGARDING DENDROGRAM PLOT

Y-AXIS PLOTTED BETWEEN 1.0 AND .4

TABLE 11. EXAMPLE OF OUTPUT FROM CLUSTER ANALYSIS (R-MODE)

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

FROM STATS PROGRAM NUMBER OF SAMPLES = 21 NUMBER OF ELEMENTS = 10

R-MODE ANALYSIS , READ "SAMPLE" AS VARIABLE. CLUSTERING BY THE WEIGHTED PAIR-GROUP METHOD USING PROPORTIONAL SIMILARITY COEFFICIENT

PRINTOUT OF DATA MATRIX

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| WANDAGEE/31457 | .0400 | 41.5300 | .1500 | 18.0200 | 8.0000 | 7.0400 | .3100 | 19.7000 | 6.9100 | .0100 |
| WANDAGEE/31458 | .0200 | 41.8000 | .4400 | 19.1800 | 5.4500 | 7.5400 | .3000 | 20.8700 | 5.5600 | .0300 |
| WANDAGEE/31460 | .0200 | 42.0900 | .2000 | 18.0400 | 6.9900 | 6.7500 | .2600 | 20.9500 | 6.1700 | .0100 |
| WANDAGEE/31461 | .0200 | 41.6000 | .2200 | 20.0300 | 4.9100 | 6.7100 | .3300 | 20.6100 | 5.9100 | .0100 |
| WANDAGEE/31462 | .0200 | 41.2400 | .3600 | 20.0000 | 4.6000 | 7.2400 | .3800 | 20.2900 | 5.5600 | .0600 |
| WANDAGEE/31463 | .0200 | 41.9400 | .1700 | 21.3900 | 3.5600 | 6.9200 | .3100 | 21.0800 | 5.4200 | .0300 |
| WANDAGEE/31464 | .0200 | 41.5900 | .3900 | 19.3900 | 5.0700 | 7.0500 | .3300 | 20.7500 | 5.8800 | .0100 |
| WANDAGEE/31465 | .0400 | 41.1600 | .4000 | 18.8800 | 5.3700 | 7.1000 | .2600 | 20.5600 | 5.9600 | .0200 |
| WANDAGEE/31466 | .0200 | 41.9300 | .5000 | 20.9900 | 2.8200 | 7.3400 | .2400 | 22.1200 | 4.8000 | .0500 |
| WANDAGEE/31467 | .0200 | 41.5500 | .4100 | 20.6500 | 3.5400 | 7.5800 | .3200 | 21.1700 | 5.3900 | .0500 |
| WANDAGEE/31468 | .0500 | 42.2900 | .2400 | 22.5000 | 1.8900 | 7.0200 | .2700 | 22.0300 | 5.0600 | .0300 |
| WANDAGEE/31476 | .0400 | 40.1100 | .1200 | 13.8500 | 11.9600 | 7.2200 | .3600 | 18.6800 | 7.6100 | .0500 |
| WANDAGEE/31477 | .0400 | 39.6100 | .0900 | 12.5700 | 13.3100 | 7.5400 | .3300 | 17.1200 | 9.2900 | .0400 |
| WANDAGEE/31478 | .0200 | 40.5800 | .4100 | 16.2600 | 8.7700 | 6.8500 | .2900 | 19.5500 | 6.8700 | .0700 |
| WANDAGEE/31479 | .0400 | 40.4800 | .3800 | 18.2200 | 6.6800 | 7.2700 | .3800 | 19.0500 | 6.7200 | .0900 |
| WANDAGEE/31480 | .0500 | 40.4400 | .3300 | 17.4600 | 8.0000 | 6.9800 | .2900 | 20.3200 | 5.8900 | .0500 |
| WANDAGEE/31481 | .0200 | 41.3100 | .1900 | 20.0100 | 5.1300 | 7.0600 | .3600 | 20.2900 | 6.2100 | .0500 |
| WANDAGEE/31482 | .0200 | 40.7100 | .4300 | 18.2600 | 6.9500 | 7.5600 | .3600 | 19.2200 | 6.8100 | .0600 |
| WANDAGEE/31483 | .0200 | 41.5600 | .2100 | 20.2700 | 4.6100 | 7.4500 | .4000 | 20.2800 | 6.0500 | .0400 |
| WANDAGEE/31484 | .0200 | 41.4100 | .4500 | 18.4200 | 6.5000 | 7.0700 | .2800 | 20.4000 | 6.2900 | .0500 |
| WANDAGEE/31485 | .0200 | 38.2800 | .0100 | 22.2200 | .0100 | 28.2300 | .8900 | 7.4000 | 3.7200 | .0300 |

**TABLE 11. continued**

VARIABLES TRANSFORMED TO PERCENT OF THEIR RANGE

PRINTOUT OF TRANSFORMED DATA MATRIX

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| WANDAGEE/31457 | .6667 | .8105 | .2857 | .5488 | .6008 | .0153 | .1077 | .8356 | .5727 | .0000 |
| WANDAGEE/31458 | .0000 | .8778 | .8776 | .6657 | .4090 | .0386 | .0923 | .9151 | .3303 | .2500 |
| WANDAGEE/31460 | .0000 | .9501 | .3878 | .5509 | .5248 | .0019 | .0308 | .9205 | .4399 | .0000 |
| WANDAGEE/31461 | .0000 | .8279 | .4286 | .7513 | .3684 | .0000 | .1385 | .8974 | .3932 | .0000 |
| WANDAGEE/31462 | .0000 | .7382 | .7143 | .7482 | .3451 | .0246 | .2154 | .8757 | .3303 | .6250 |
| WANDAGEE/31463 | .0000 | .9127 | .3265 | .8882 | .2669 | .0098 | .1077 | .9293 | .3052 | .2500 |
| WANDAGEE/31464 | .0000 | .8254 | .7755 | .6868 | .3805 | .0158 | .1385 | .9069 | .3878 | .0000 |
| WANDAGEE/31465 | .6667 | .7182 | .7959 | .6354 | .4030 | .0181 | .0308 | .8940 | .4022 | .1250 |
| WANDAGEE/31466 | .0000 | .9102 | 1.0000 | .8479 | .2113 | .0293 | .0000 | 1.0000 | .1939 | .5000 |
| WANDAGEE/31467 | .0000 | .8155 | .8163 | .8137 | .2654 | .0404 | .1231 | .9355 | .2998 | .5000 |
| WANDAGEE/31468 | 1.0000 | 1.0000 | .4694 | 1.0000 | .1414 | .0144 | .0462 | .9939 | .2406 | .2500 |
| WANDAGEE/31476 | .6667 | .4564 | .2245 | .1289 | .8985 | .0237 | .1846 | .7663 | .6984 | .5000 |
| WANDAGEE/31477 | .6667 | .3317 | .1633 | .0000 | 1.0000 | .0386 | .1385 | .6603 | 1.0000 | .3750 |
| WANDAGEE/31478 | .0000 | .5736 | .8163 | .3716 | .6586 | .0065 | .0769 | .8254 | .5655 | .7500 |
| WANDAGEE/31479 | .6667 | .5486 | .7551 | .5690 | .5015 | .0260 | .2154 | .7914 | .5386 | 1.0000 |
| WANDAGEE/31480 | 1.0000 | .5387 | .6531 | .4924 | .6008 | .0125 | .0769 | .8777 | .3896 | .5000 |
| WANDAGEE/31481 | .0000 | .7556 | .3673 | .7492 | .3850 | .0163 | .1846 | .8757 | .4470 | .5000 |
| WANDAGEE/31482 | .0000 | .6060 | .8571 | .5730 | .5218 | .0395 | .1846 | .8030 | .5548 | .6250 |
| WANDAGEE/31483 | .0000 | .8180 | .4082 | .7754 | .3459 | .0344 | .2462 | .8750 | .4183 | .3750 |
| WANDAGEE/31484 | .0000 | .7805 | .8980 | .5891 | .4880 | .0167 | .0615 | .8832 | .4614 | .5000 |
| WANDAGEE/31485 | .0000 | .0000 | .0000 | .9718 | .0000 | 1.0000 | 1.0000 | .0000 | .0000 | .2500 |

**TABLE 11 continued**

FROM STATS PROGRAM

CLUSTERING BY THE WEIGHTED PAIR-GROUP METHOD

| SAMPLE NUMBERS | | LEVEL OF ASSOCIATION | CYCLE NUMBER |
|---|---|---|---|
| 2 | 8 | .9387 | 1 |
| 5 | 9 | .9708 | 1 |
| 6 | 7 | .9742 | 1 |
| 2 | 3 | .7423 | 2 |
| 5 | 1 | .6736 | 2 |
| 6 | 4 | .6386 | 2 |
| 5 | 10 | .5563 | 3 |
| 5 | 2 | .4971 | 4 |
| 5 | 6 | .3650 | 5 |

FROM STATS PROGRAM

ORDER OF SAMPLES FOR DENDROGRAM PLOT

| | |
|---|---|
| Cr2O3 | 5 |
| CaO | 9 |
| P2O5 | 1 |
| Na2O | 10 |
| SiO2 | 2 |
| MgO | 8 |
| TiO2 | 3 |
| FeO | 6 |
| MnO | 7 |
| Al2O3 | 4 |

FROM STATS PROGRAM

INFORMATION REGARDING DENDROGRAM PLOT

Y-AXIS PLOTTED BETWEEN 1.0 AND .3

# 11 BMRDEND (DENDOGRAMS FOR CLUSTER ANALYSIS)

Dendograms of the cluster analysis generated by program CLUSTA may be dis played using program BMRDEND, which is invoked by typing BMRDEND or option 8 of the GDA-MDA menu. The dendograms may be displayed on screen or output to a plot metafile (GDA1.VEC to GDA99.VEC). The metafiles may be output to a printer or HP-compatible plotter using the VECTOR program.

Examples of the dendograms generated from the cluster analysis of a suite of garnets from heavy mineral concentrate from the Wandagee alkaline intrusions are given in Figures 6A and 6B.

Figure 6A is an example of Q-mode using the correlation coefficient with no weightings. The cluster analysis generates similar groupings to that of Dawson and Stephens (1975) in that groups 5 (magnesian almandine), 10 (low-calcium chrome-pyrope), 12 (knorringitic uvarovite-pyrope) are clearly separated, and most group 1 (titanium pyrope), group 11 (uvarovite-pyrope) and group 9 (chrome-pyrope) garnets are clustered. This analysis also recognises a high correlation between chrome-bearing titanian pyropes and groups 9 and 11.

Figure 6B is an example of R-mode cluster analysis using the proportional similarity coefficient.

FIG. 6A. Q–MODE DENDOGRAM OF GARNET COMPOSITIONS

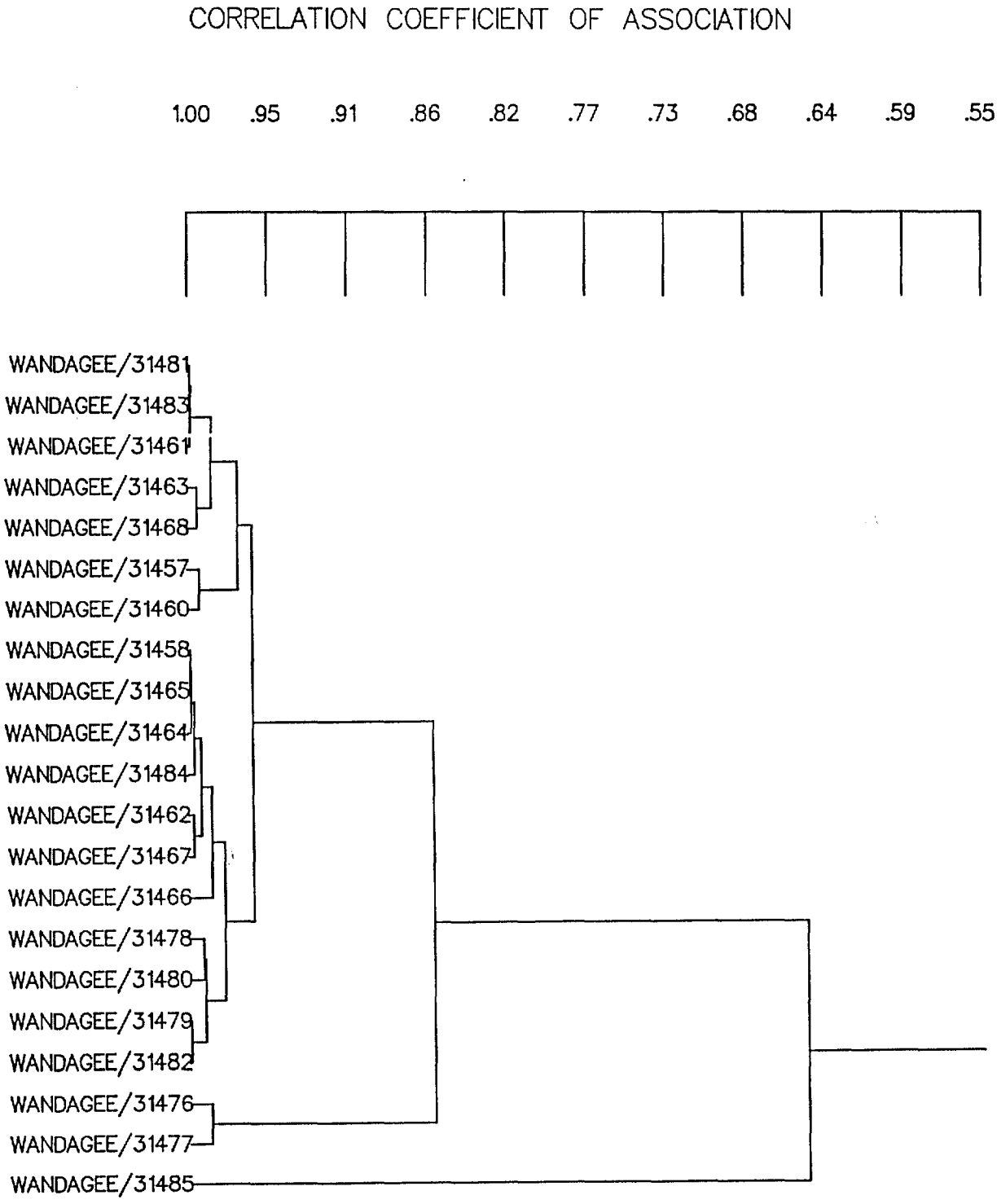
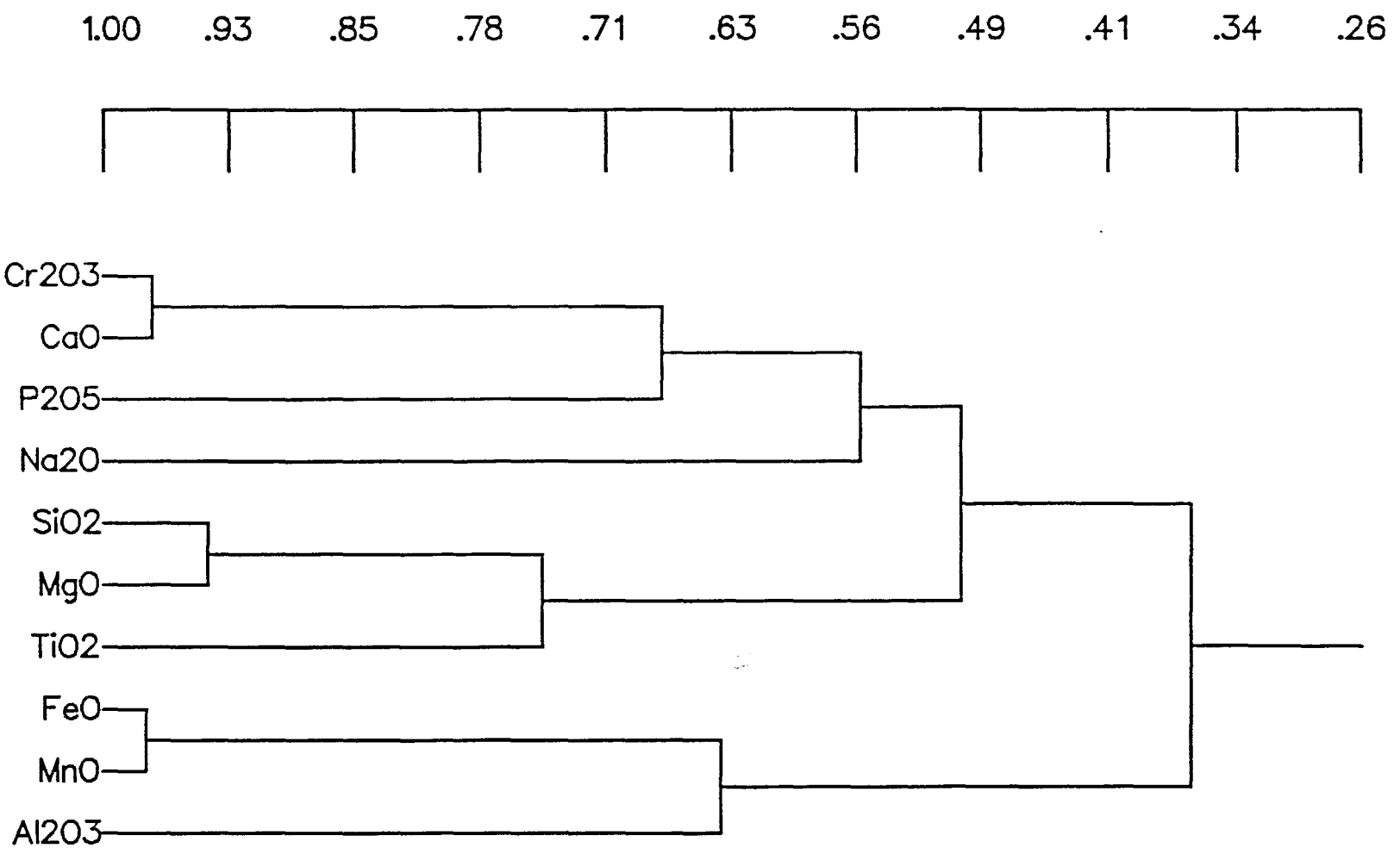


FIG. 6B. R–MODE DENDOGRAM OF GARNET COMPOSITIONS

PROPORTIONAL SIMILARITY COEFFICIENT



# 12 UTIL (UTILITIES PROGRAM)

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 and data entered through ENTMIN can be edited prior to conversion to GDA files, 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, or selecting option 1 of the combined GDA- MDA menu. The UTIL menu is as follows:

(1) Create a new file
(The fields (maximum of 15 element or oxide concentration fields) on the new datafile are defined by a utilities field names file, such as OXIDE.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 anlyses
(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; previously entered data are retained, unless changed).

(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 in upper or lower case; for concentration data, samples must be re-assigned before any added data can be plotted; in either case, the report definition file (MINREPT.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) Write group(s) to a new file.
(Selected groups can be written from an existing GDA file to a new GDA file).

(16) Display structural formulae, normalise minerals

The default utilities field names file is UTIL.UTL, which includes all the standard GDA descriptive fields and elements. Minerals applications should select OXIDE.UTL or METAL.UTL as appropriate. 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, may be entered (although obviously such data will not be convertible into structural formulae, mineral end-members, etc.). The maximum number of numerical (concentration) fields for mineral applications is 15.

# 13 SUMMARY

1. The first step in using the GDA-MDA system is to get analytical data (including mineral analyses) in the form of datafiles (GDA files) suitable for processing. There are several ways of doing this. Mineral analyses may be entered directly using the ENTMIN program or, alternatively, data from a database (such as ORACLE) can be entered into the system on ASCII files. Such files must be transformed into GDA files using the **ORACLE** program. Alternatively, 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 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 mineral, lithology, or locality. 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 (BMRMDA, VECTOR, TABMIN, STATS, CLUSTER).

4. The main minerals analysis program (**BMRMDA**) enables generation of plots, initially on the PC screen, and then as plot metafiles for output to plotters or other devices, and preparation of tables of analyses. Firstly, data (element concentrations, cations calculated from structural formulae, end-member molecules or any derived arithmetic ratio) are extracted into datasets. The selected datasets are used to produce histograms, XY plots, triangular plots, or box-whisker plots. The required plots are then written to metafiles for subsequent output. Facilities also exist for classification and naming of certain minerals (pyroxenes, amphiboles, garnets, spinels), and for plotting of spinel compositions in the reduced or oxidized spinel prisms. **BMRMDA** also has the facility to generate tables of structural formulae.

5. Output of plot metafiles to plotters, printers, or screen is carried out by the **VECTOR** program. Some types of plot file may also be copied directly to laser printers, or used as input to word processing systems. VECTOR includes facilities for positioning plots on a page.

6. **TABMIN** allows printing of tables of mineral analyses including both major and trace element data, structural formulae, and element ratios or other derived values. 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. A program **OUTGDA** can be used to write analyses from GDA to ASCII files for input to other systems or databases.

# 14 ACKNOWLEDGEMENTS

The bulk of the programs in the GDA-MDA system were written at BMR. However, several of the MDA applications either incorporate specific routines or were developed from base programs written by others. We particularly thank the following individuals for generously making available programs/routines for adaption and incorporation into the system: Nick Ware, Wayne Taylor, Rod Ryburn, Nick Rock, and Ken Currie. We also thank Peter Williams for advice, and Julie Haldane for preparation of this manual for printing.

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# APPENDIX A — SYSTEM LIMITATIONS

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

| Max | Description |
|---|---|
| 50 | number of groups |
| 11 | number of datasets (BMRGDA) |
| 4 | number of datasets (BMRMDA) |
| 800 | number of assigned samples (BMRGDA) |
| 400 | number of assigned samples (BMRMDA) |
| 15 | number of symbols |
| 8 | number of plotter pens |
| 6 | 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 |
| 30 | number of elements in a box-whisker plot |
| 100 | number of bars in a histogram |
| 20 | number of sample numbers typed in for spidergram |
| 15 | number of columns in report |
| 800 | number of samples for least squares line fit (BMRGDA) |
| 0 | number of samples for least squares line fit (BMRMDA) |
| 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 |
| 50 | number of characters of text for added plot points or text |
| 20 | number of additional plot points and/or text lines |

# APPENDIX B — PARAMETER FILES

Various types of parameter file are available for use in entering data or expressions, defining output, plots etc. New files may be set up as required, provided the format of the given file type is adhered to, or any of the existing ones may be edited (e.g., using WORDSTAR non-document mode). Numbers after the major element, trace element, and description field title lines in the .MTB and .RPT files give the number of lines (fields) in each of these three groups.

The GDA manual gives examples of the various parameter files used in extracting data in the BMRGDA program. The main parameter files used for MDA are:

OXIDE.DEF – defines concentration fields for processing purposes, and contains the element to oxide conversion factors for most of the periodic table; used for analyses of silicates and oxides.

METAL.DEF – similar to OXIDE.DEF, but contains only elements, and is used for analyses of metals and sulphides.

OXIDE.MTB – report definition file used to define output (e.g., change field names, define major and trace elements)in TABMIN; used for oxide and silicate analyses.

METAL.MTB – similar to OXIDE.MTB, but used for metal and sulphide analyses.

OXIDE.RPT – report definition file containing some 23 common major elements (as oxides) to be used in generating tables of analyses (without structural fomulae) using TABLE. Also used in STATS.

METAL.RPT – similar to MINREPT.RPT, but used for metal and sulphide analyses.

OXIDE.UTL – utilities field names file used in UTIL to define the descriptive and element concentration fields for new GDA files containing oxide and silicate analyses.

METAL.UTL – similar to OXIDE.UTL, but used for metal and sulphide analyses.

To avoid confusion and to enable a listing when the ? = prompt appears, it is recommended that any new files are named according to the nomenclature above. OXIDE.DEF, OXIDE.MTB, MINREPT.RPT, and OXIDE.UTL are given in the following pages.

PARAMETER FILE OXIDE.DEF

Probe analysis data defn (atomic no, element, oxide, oxide factor) OXIDE.DEF

| | | |
|---|---|---|
| 03 | Li Li2O | 1.47304 |
| 04 | Be BeO | 2.77530 |
| 05 | B B2O3 | 3.21987 |
| 06 | C CO2 | 3.66409 |
| 07 | N NO3 | 4.42680 |
| 08 | O Owt | 1.0 |
| 09 | F Fwt | 1.0 |
| 10 | Ne Newt | 1.0 |
| 11 | Na Na2O | 1.34797 |
| 12 | Mg MgO | 1.65807 |
| 13 | Al Al2O3 | 1.88946 |
| 14 | Si SiO2 | 2.13932 |
| 15 | P P2O5 | 2.29137 |
| 16 | S SO3 | 2.49694 |
| 17 | Cl Clwt | 1.0 |
| 18 | Ar Arwt | 1.0 |
| 19 | K K2O | 1.20458 |
| 20 | Ca CaO | 1.39920 |
| 21 | Sc Sc2O3 | 1.53384 |
| 22 | Ti TiO2 | 1.66806 |
| 23 | V V2O3 | 1.47919 |
| 24 | Cr Cr2O3 | 1.46155 |
| 25 | Mn MnO | 1.29122 |
| 26 | Fe FeO | 1.28648 |
| 27 | Co CoO | 1.27148 |
| 28 | Ni NiO | 1.27262 |
| 29 | Cu CuO | 1.25181 |
| 30 | Zn ZnO | 1.24476 |
| 31 | Ga Ga2O3 | 1.34423 |
| 32 | Ge GeO2 | 1.44083 |
| 33 | As As2O3 | 1.32032 |
| 34 | Se Sewt | 1.0 |
| 35 | Br Brwt | 1.0 |
| 36 | Kr Krwt | 1.0 |
| 37 | Rb Rb2O | 1.09360 |
| 38 | Sr SrO | 1.18261 |
| 39 | Y Y2O3 | 1.26994 |
| 40 | Zr ZrO2 | 1.35080 |
| 41 | Nb Nb2O5 | 1.43053 |
| 42 | Mo MoO3 | 1.50031 |
| 44 | Ru Ruwt | 1.0 |
| 45 | Rh Rhwt | 1.0 |
| 46 | Pd Pdw | 1.0 |
| 47 | Ag Agwt | 1.0 |
| 48 | Cd Cdwt | 1.0 |

| | | |
|---|---|---|
| 49 | In Inwt | 1.0 |
| 50 | Sn SnO | 1.13480 |
| 51 | Sb Sbwt | 1.0 |
| 52 | Te Tewt | 1.0 |
| 53 | I Iwt | 1.0 |
| 54 | Xe Xewt | 1.0 |
| 55 | Cs Cs2O3 | 1.06019 |
| 56 | Ba BaO | 1.11648 |
| 57 | La La2O3 | 1.17277 |
| 58 | Ce Ce2O3 | 1.17128 |
| 59 | Pr Pr2O3 | 1.17032 |
| 60 | Nd Nd2O3 | 1.16639 |
| 62 | Sm Sm2O3 | 1.15962 |
| 63 | Eu Eu2O3 | 1.15793 |
| 64 | Gd Gd2O3 | 1.15262 |
| 65 | Tb Tb2O3 | 1.15101 |
| 66 | Dy Dy2O3 | 1.14770 |
| 67 | Ho Ho2O3 | 1.14551 |
| 68 | Er Er2O3 | 1.14349 |
| 69 | Tm Tm2O3 | 1.14206 |
| 70 | Yb Yb2O3 | 1.13869 |
| 71 | Lu Lu2O3 | 1.13716 |
| 72 | Hf Hf2O3 | 1.17929 |
| 73 | Ta Ta2O5 | 1.22105 |
| 74 | W WO2 | 1.17405 |
| 75 | Re Rewt | 1.0 |
| 76 | Os Oswt | 1.0 |
| 77 | Ir Irwt | 1.0 |
| 78 | Pt Ptwt | 1.0 |
| 79 | Au Auwt | 1.0 |
| 80 | Hg Hgwt | 1.0 |
| 81 | Tl Tlwt | 1.0 |
| 82 | Pb PbO | 1.07723 |
| 83 | Bi Biwt | 1.0 |
| 90 | Th ThO2 | 1.13790 |
| 92 | U U3O8 | 1.17925 |

PARAMETER FILE OXIDE.MTB

Report definiton file OXIDE.MTB
Major elements
63
U3O8
MoO3
P2O5
Nb2O5
Ta2O5
SiO2

TiO2
GeO2
ZrO2
WO2
ThO2
B2O3
Al2O3
Sc2O3
V2O3
Cr2O3
Ga2O3
As2O3
Y2O3
Cs2O3
La2O3
Ce2O3
Pr2O3
Nd2O3
Sm2O3
Eu2O3
Gd2O3
Tb2O3
Dy2O3
Ho2O3
Er2O3
Tm2O3
Yb2O3
Lu2O3
Hf2O3
Fe2O3
FeO
MnO
NiO
MgO
CoO
CuO
ZnO
CaO
SrO
BaO
PbO
Li2O
Na2O
K2O
Rb2O
O
F
Ne
Cl

Ar
Br
Kr
I
Xe
CO2
NO3
SO3
Trace elements
63
U
Mo
P
Nb
Ta
Si
Ti
Ge
Zr
W
Th
B
Al
Sc
V
Cr
Ga
As
Y
Cs
La
Ce
Pr
Nd
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu
Hf
Fe
Fe3+
Fe2
Mn

Ni
Mg
Co
Cu
Zn
Ca
Sr
Ba
Pb
Li
Na
K
Rb
F
Ne
Cl
Ar
Br
Kr
I
Xe
C
N
S
Description fields
7

| | |
|---|---|
| SAMPNO | Sample number |
| ANALNO | Analysis number |
| MINERAL | Mineral name |
| MINDERSCR | Description |
| LITHOLOGY | Lithology |
| GRAINFORM | Mineral form |
| POINT | Analysis point |

PARAMETER FILE OXIDE.RPT

Report definition file OXIDE.RPT
Major Elements
23

| | |
|---|---|
| P2O5 | P2O5 |
| NB2O5 | Nb2O5 |
| ZRO2 | ZrO2 |
| SIO2 | SiO2 |
| TIO2 | TiO2 |
| AL2O3 | Al2O3 |
| CR2O3 | Cr2O3 |
| V2O3 | V2O3 |
| Y2O3 | Y2O3 |

| | |
|---|---|
| FE2O3 | Fe2O3 |
| FEO | FeO |
| MNO | MnO |
| NIO | NiO |
| CUO | CuO |
| ZNO | ZnO |
| MGO | MgO |
| CAO | CaO |
| SRO | SrO |
| BAO | BaO |
| NA2O | Na2O |
| K2O | K2O |
| F | F |
| CL | Cl |

Trace elements
0
Description fields
9

| | |
|---|---|
| SAMPNO | Sample number |
| ANALNO | Analysis number |
| MINERAL | Mineral |
| MINDESCR | Mineral description |
| LITHOLOGY | Lithology |
| GRAINFORM | Mineral form |
| POINT | Analysis point |
| OXYGENS | Number of oxygens |
| CATIONS | Number of cations |

PARAMETER FILE OXIDE.UTL

Utilities field names file OXIDE.UTL
Description Fields
SAMPNO
ANALNO
MINERAL
MINDESCR
LITHOLOGY
GRAINFORM
POINT
OXYGENS
CATIONS
Element Fields
P2O5
SIO2
TIO2
AL2O3
CR2O3
FE2O3

FEO
MNO
NIO
MGO
CAO
BAO
NA2O
K2O
S

# APPENDIX C — GRAPHICS OVERLAY FILES

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

The format of a typical .GRF file is as follows:

```
Graphics overlay file - TSTGDA.GRF
*
* example file
*
*
Font          11
Pen           4
Textsize
0.5
Text
Aa Bb Cc 1234567890
    68.0    0.9
*
Pen           5
Linetype      4
Line          3
68.0  0.2
70.0  0.5
74.0  0.8
Pen           2
Linetype      2
Line          2
68.0  0.2
99.0  0.4
*
Linetype      1
Pen           3
Symbolsize
2.0
Symbol        6
70.0  0.5
```

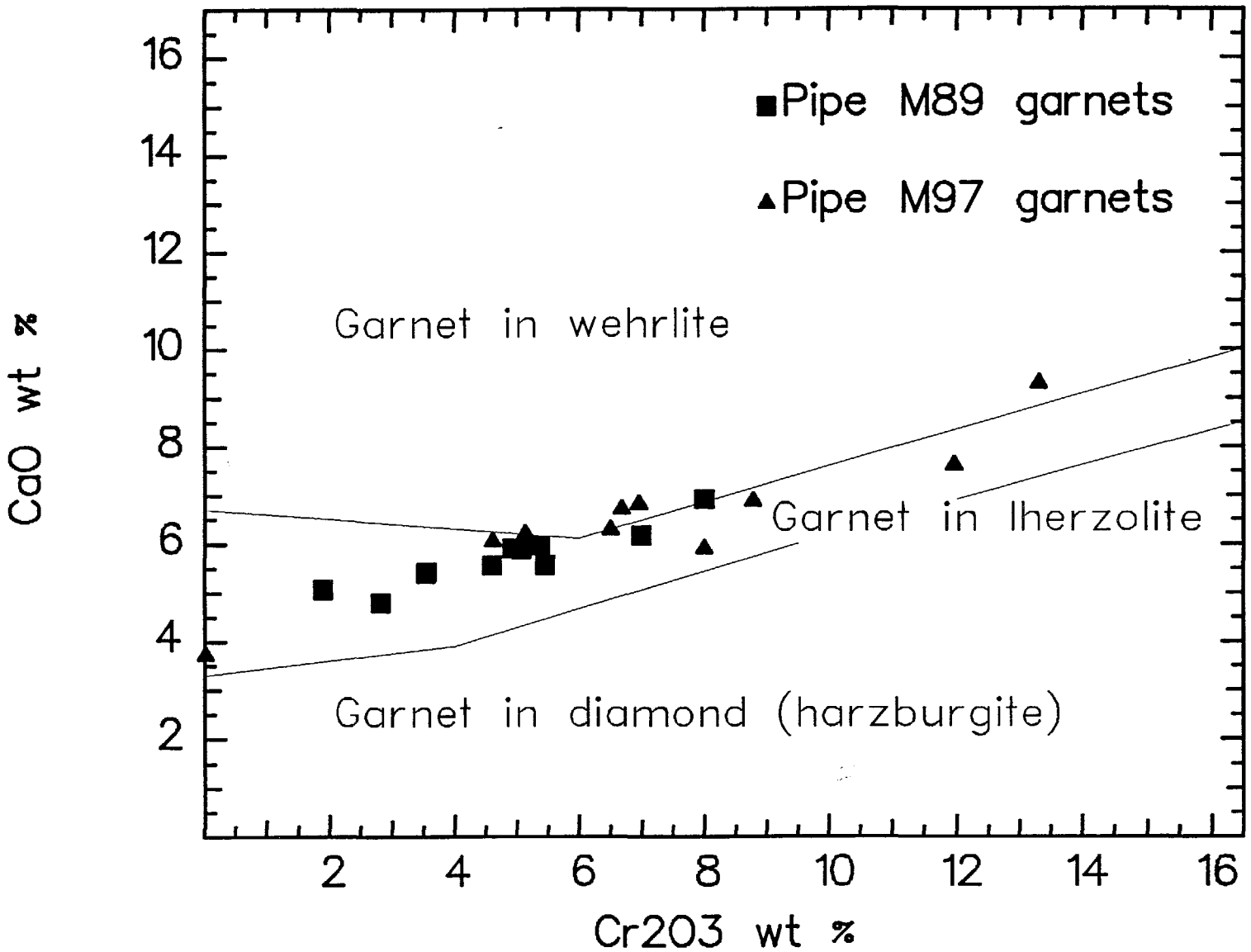
The first line, which specifies the file type, is mandatory, and any lines beginning with a * are used for explanatory comments. Text can be displayed by specifying font, pen colour, and textsize, followed by the text itself and the XY co-ordinates of the beginning of the text. Symbols require pen colour, symbol size 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, text size, and symbol size 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 (symbol size and text size) 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.

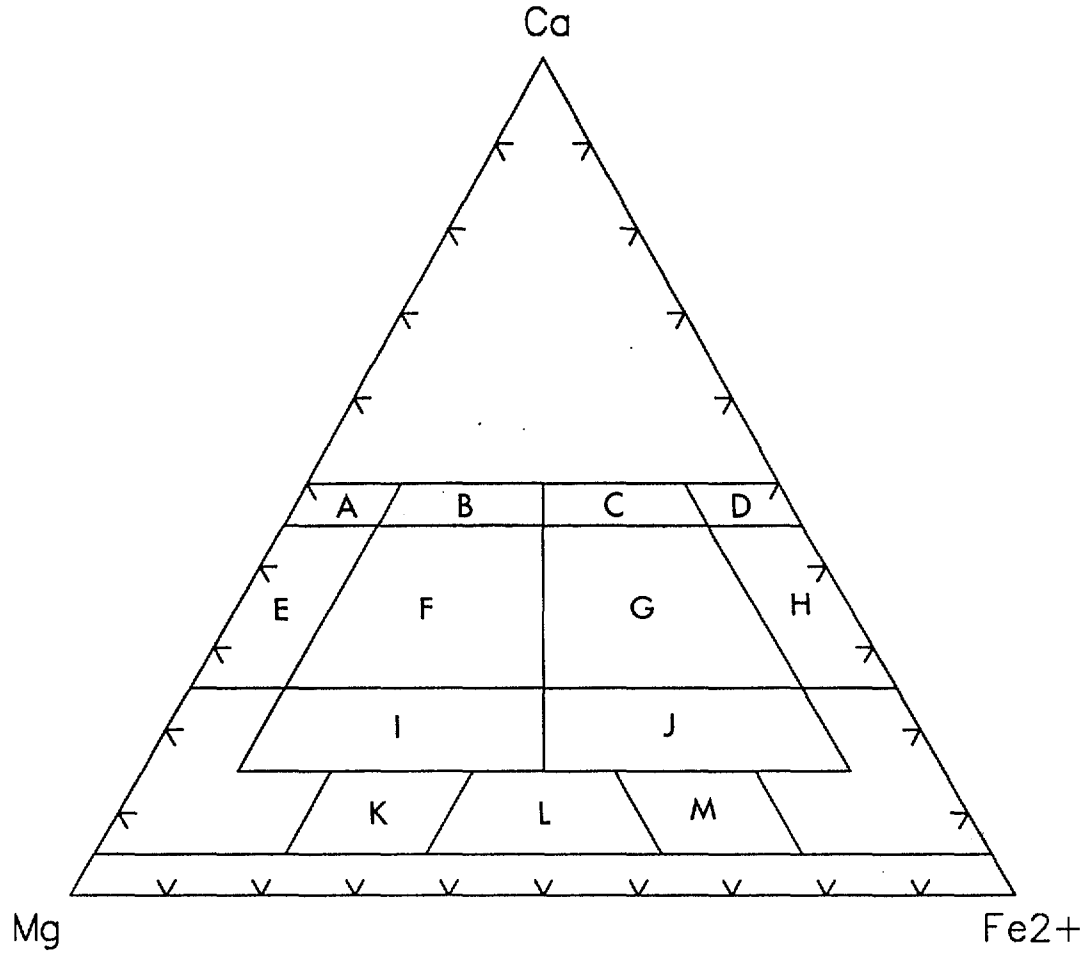
An example of a graphics overlay file (GARSOB.GRF) used to discriminate mantle garnets on a w% $Cr_2O_3$ versus CaO diagram (Sobolev et al., 1973) is given below and its application shown in Figure 7. The clinopyroxene classification of Poldervaart & Hess (1951) (PYROXENE.GRF) is given in Figure 8, and further examples of graphics overlay files (mostly for whole-rock data) are given in the GDA manual. Note all use the extension .GRF. In many cases text has not been included in the files to avoid superimposing text on plot points.

```
Graphics overlay file - GARSOB.GRF
*Cr203-CaO garnet discrimination diagram
*after Sobolev et al (1973, CMP 40, 39-52)
Font        6
Pen         6
Textsize
1.0
Text
Garnet in diamond (harzburgite)
2.0,2.0
Text
Garnet in wehrlite
2.0,10.0
Text
Garnet in lherzolite
1.0,5.0
Linetype    1
Line        2
0.0,3.3
4.0,3.9
Line        2
4.0,3.9
16.5,8.5
Line
0.0,6.7
6.0,6.1
Line        2
6.0,6.1
16.5,10.0
```

FIG. 7. XY PLOT OF GARNETS WITH GRAPHICS OVERLAY FILE



```
Graphics overlay file - PYROXENE.GRF
*Classification of clinopyroxenes:
*Poldervaart & Hess (1951)
Pen         1
Linetype    1
Line        2
50.0,50.0
0.0,50.0
Line        2
55.0,45.0
0.0,45.0
Line        2
75.0,25.0
0.0,25.0
Line        2
95.0,5.0
0.0,5.0
Line        2
25.0,50.0
42.5,15.0
Line        4
40.0,50.0
75.0,15.0
10.0,15.0
10.0,50.0
Line        2
65.0,15.0
75.0,5.0
Line        2
50.0,15.0
60.0,5.0
Line        2
35.0,15.0
35.0,5.0
Line        2
20.0,15.0
20.0,5.0
```




PYROXENE.GRF (Poldervaart & Hess, 1951)

A. Diopside
B. Salite
C. Ferrosalite
D. Hedenbergite
E. Endiopside
F. Augite
G. Ferroaugite
H. Ferrohedenbergite
I. Subcalcic augite
J. Subcalcic ferroaugite
K. Magnesium pigeonite
L. Intermediate pigeonite
M. Ferriferous pigeonite

FIG. 8