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AUSTRALIA

MINERAL DATA ANALYSIS SYSTEM REFERENCE MANUAL

RECORD 90/91
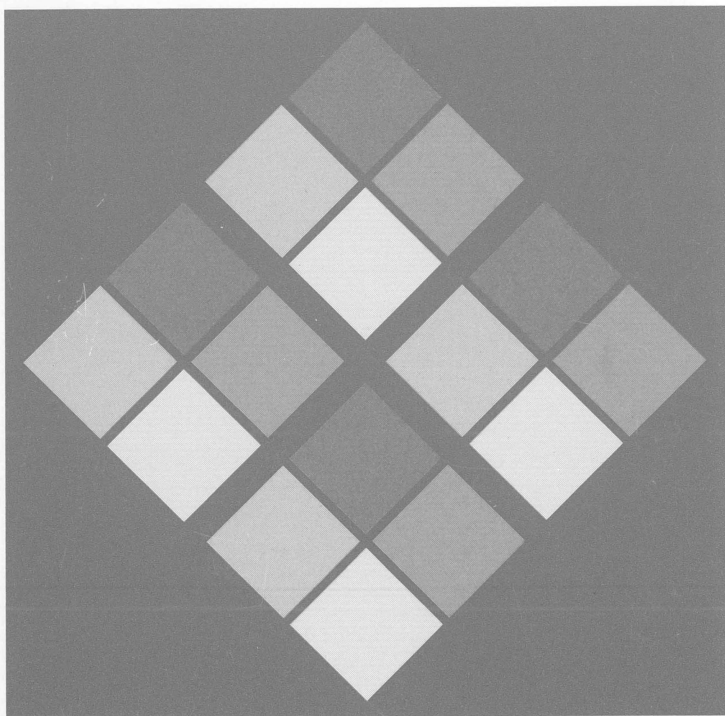
by A.L. Jaques, L. Simons and J.W. Sheraton

Bureau of Mineral Resources, Geology and Geophysics

Record 1990/91

MINERAL DATA ANALYSIS SYSTEM (MDA)

REFERENCE MANUAL

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A.L. Jaques, L. Simons and J.W. Sheraton

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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

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Enquiries regarding purchase of the system should be made to the BMR Publication Sales at the same address (phone (06) 2451374, fax (06) 2472728).

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 Record 1988/45), BMR's comprehensive PC-based system for processing whole-rock geochemical data. The programs are written in FORTRAN 77 (Microsoft compiler) and use a graphics package (Media Cybernetics HALO) 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. Other programs allow samples to be assigned to groups for plotting purposes, and editing and merging of datafiles.

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 any program 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.

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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 data base, processing, the generation of plots (histograms, XY plots, triangular plots) and the calculation of statistical functions, but includes a number of programs which are specific to mineral chemical analyses. The programs permit transfer of mineral analyses from the electron proble microanalyser (EPMA), 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 1988/45) 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 ten sub-programs which are incorporated into three main programs - ENTMIN, MDAPROG and TABMIN. MDA also uses nine 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 invoked 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.

DEND - 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.

MDAPROG - the core program of MDA containing 23 sub-programs. These enable 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; analysis of the datasets including previews on the PC screen, and outputing 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 database (e.g., ORACLE) or for export and/or processing by other systems.

PLOT - outputs graphics metafiles (from MDA and GDA) to a plotter or HPGL file.

PROBE - this program accepts mineral data on ASCII files from the ANU/BMR Cameca electron probe micro analyser (EPMA) and creates and ORACLE format file. It is not included in the main GDA-MDA menu and must be run by typing PROBE.

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. 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 = Assign large numbers (>800) of samples to groups (BIGASS)

5 = Output to plotter / HPGL printer (PLOT)

6 = Statistical functions (STATS)

7 = Cluster analysis (CLUSTA)

8 - Dendrograms for cluster analysis (DEND)

9 - Export GDA file as ASCII file (OUTGDA)

*** GEOCHEMICAL - GDA ONLY ***

10 - Geochemical data analysis (GDAPROG)

11 - Geochemical data analysis for >800 samples (BIGGDA)

12 - Geochemical data analysis for >11 datasets (SMALLGDA)

13 - Generate tables of analyses (TABLE)

14 - Petrological modelling (PETMOD)

*** MINERALS - MDA ONLY ***

15 = Enter mineral data from keyboard (ENTMIN)

16 = Minerals data analysis (MDAPROG)

17 = Generate tables of anlyses (TABMIN)

1.2 Parameter Files

System parameters, each as element to oxide conversion factors, are held on
files which can be modified with a text editor or word processor (e.g.,
WORDSTAR non-document mode). Some files are generated during processing and
can also be modified. Care must be taken to preserve the format (logical
structure) of the files. The first line of a file must not be changed as it
is used to specify the type of file.

1.3 Printouts

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

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) 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). Media
Cybernetics HALO 88 is used for graphics to provide support for HP plotters
and several displays (EGA, Hercules, and VGA, but note that earlier versions
of HALO do not support VGA).

1.6 Hardware Requirements

An IBM PC or compatible is required with 640K RAM, a 10 megabyte hard disk
(the actual GDA and MDA programs require about 6 MB, and an additional 1 MB
with source code), and a Hercules, EGA, or VGA colour graphics card. A HP
compatible plotter is required for hardcopy graphics and a printer for
reports. Plot files can be converted to HPGL files and output to a Laser
printer.

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. In the case of data obtained on the ANU/BMR EPMA, a unique 5 digit analysis number is set by the EPMA software.

The data can be extracted from an existing database, transferred from EPMA in the form of an ASCII file (eg., using program PROBE) 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 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 (MDA, PROG, PLOT, TABMIN, STATS, and 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 5¼" or 3½" format. The MDA and GDA systems may be built up from the FORTRAN source code if Microsoft FORTRAN 77 and HALO are also installed, and details are given in Appendix B. Alternatively, if the compiled version is available, it is only necessary to carry out the following steps:

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

2.   Copy the contents of all the floppy disks to the GDA directory; (if GDA is already on the hard disk copy only the additional MDA programs and files);

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

     EGA.DEV   - the EGA driver

     HERC.DEV   - the Hercules driver

     VGA.DEV   - the VGA driver

the other files can be deleted;

4.   Edit the file SITE.DEF as described in the GDA Manual (BMR Record 1988/45, pages 6-7) to specify the appropriate graphics card for your system (EGA, VGA or HERC (model 1);

5.   Copy the new version of GDA.MENU or edit the existing version to incorporate MDA programs in the menu.

3. DATA ENTRY

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

3.1 From Microprobe

Data may be transferred direct from ASCII file output from the electron probe microanalyser to the GDA/MDA system using program PROBE. Full details of the ANU/BMR system are given in Appendix E.

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).
- 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.
- Data are then entered in turn until all the oxide or element fields are filled.

NOTE: If several sessions are required to enter a dataset each session should use a different .ORC file as ENTMIN overwrites and does not append files of the same name. Files can be concatonated 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 number (SAMPNO's) 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	AL203	SIO2	CAO	TIO2	V203	CR203
MNO	FEO	NIO				

Enter values for next analysis

Wt % for SIO2	(zero):	.13
Wt % for TIO2	(zero):	2.62
Wt % for AL203	(zero):	3.32
Wt % for CR203	(zero):	54.56
Wt % for V203	(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
Al203	3.32	0.1372	17571
SiO2	.13	.0046	608
CaO	.07	.0026	500
TiO2	2.62	.0691	15707
V203	.07	.0020	476
Cr203	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)?

3.3   Extraction From Oracle Database

Data may be extracted from the (Oracle) database in ASCII format. Full
details of this procedure are given on pages 8 to 11 in the GDA manual (BMR
Record 1988/45).

4. ORACLE

Data entered into the system in Oracle format (i.e., 80 character ASCII files) must be converted into an internal (GDA) file 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 data base does not have to be used.

The file consists of records 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. An example is given below of an ASCII file in Oracle format.

```
ANALNO
- - - - - - - -
SAMPNO
- - - - - - - -
MINERAL
- - - - - - - - - - - - - - - - - - - - - - - - - - -
MINDESCR
- - - - - - - - - - - - - - - - - - - - - - - - - - -
STRATUNIT
- - - - - - - -
OXYGENS
- - - - - - - -
CATIONS
- - - - - - - -
SIO2
- - - - - - - -
NA20
- - - - - - - -
MGO
- - - - - - - -
AL203
- - - - - - - -
P205
- - - - - - - -
K20
- - - - - - - -
CAO
- - - - - - - -
TIO2
- - - - - - - -
CR203
```

```
----------
MNO
----------
FEO
----------
NIO
----------
NA
----------
MG
----------
AL
----------
SI
----------
P
----------
K
----------
CA
----------
TI
----------
CR
----------
MN
----------
FE
----------
NI
----------
31457
WANDAGEE
GARNET CONCENTRATE M97
GEN 256 GARNET 002
PIPE M97
    12.00
      .00
 41.5310
   -.0198
 19.6979
 18.0241
    .0376
   -.0122
   6.9150
    .1536
   7.9976
    .3071
   7.0444
   -.0354
    .0000
    .0000
    .0000
    .0000
    .0000
    .0000
    .0000
    .0000
    .0000
    .0000
    .0000
    .0000
```

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. Subsequent fields are taken as containing numerical data. With this proviso, the actual order within each set of fields (i.e., descriptive and concentration) is immaterial. A concentration of zero means that there is no value for that element. When an element concentration is below the detection limit, the value given is the negative of the detection limit. The value used in processing will be half the positive value. All field names are held internally in upper case to simplify comparisons, but can be redefined for the report programs.

The program is run by typing ORACLE 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).

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 and unless otherwise specified the standard .ORC and .GDA file extensions are applied.

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.

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. 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, MINERAL DESCRIPTION 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; 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 the samples to the group.

The logic is typed in as lines, where each line is an 'or' condition. A maximum of 10 lines (ie., 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., other data) 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), named, 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). This logic will extract all Wandagee chromites into group 1, chromites from Wandagee pipe M97 into group 2, all Wandagee garnets into group 3 and all Wandagee garnets excluding these from pipe M89 into group 4.

Global logic

SAMPNO == WANDAGEE

Group number 1

WANDAGEE CHROMITES

MINERAL == CHROMITE

Group number 2

PIPE M97 CHROMITES

MINERAL == CHROMITE && STRATUNIT == PIPE M97

Group number 3

WANDAGEE GARNETS

MINERAL == GARNET

Group number 4

GARNETS EX M89

MINERAL == GARNET && STRATUNIT != PIPE M89

The assignment of samples into the specified groups may be printed out from
the file ASSIGN.PRN. Further details of assignment procedures are given in
the GDA manual.

6. MDAPROG

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 options are selected from the menu of the MDA program which is run by typing MDAPROG or option 16 on the main GDA-MDA menu. A GDA file name (as generated in the ORACLE program) must then be specified (if using a floppy disc the drive must be specified eg. A:xyz) and also the mineral definition file, either OXIDE.DEF or METAL.DEF depending on whether the data are as oxide or element concentrations.

The MDA menu is 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.PLT 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 (non-document mode) prior to printing.

For .graphical display/analysis the first step is to extract data, either the stored oxide/element concentrations or information calculated from this, such as cations, end-member components, cation ratios, etc., from the GDA file for plotting. Data are extracted into data sets (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 prism. 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 PLOT 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.

The following example extracts from a set of chromite analyses the Cr_2O_3

and MgO contents (data sets 1 and 2), the Al_2O_3 + Fe_2O_3 content (data

set 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)

: **CR2O3**

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 data sets) followed by the DATA SET 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 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:

$$(FE_2O_3 + FEO)/2 > 50 < 90.0$$

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 elemental concentrations in the GDA file. The program calculates structural formulae on the basis of the number of cations and oxygens specified in the GDA file. An option is available to specify calculation with or without ferric iron.

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

Type arithmetic expression [?=help] (Exit)

: 100*Cr/(Cr+Al)

Data set number [1 - 4]: 1

Type arithmetic expression [?=help] (Exit)

: 100*Mg/(Mg+Fe2+)

Data set number [1 - 4]: 2

Type arithmetic expression [?=help] (Exit)

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

Data set number [1 - 4]: 3

Type arithmetic expression [?=help] (Exit)

: Cr/(Cr+Al+Fe3+)

Data set number [1 - 4]: 4

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

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 stored and later renamed to 'Mol percent Or' or similar using options provided under the plotting routines.

Extraction of combined oxide or elemental weight percent data or other parameters such as stratigraphic height or with 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 MDAPROG 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 = $Al(M1)+Cr+Fe^{3+}+2Ti$

ln(a)En   =   log activity enstatite

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

The program alo 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(M1)	Mg(M1)	(ACF2T)	T(tot)	M1(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. Options enable estimation by either normalising cations exclusive of Ca, Na, and K to 13, i.e., T + C = 13, or by normalising the T + C + B exclusive of Na and K to 15 cations. 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.

Mineral 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.

$$Mg\# \quad = \quad 100\ Mg/(Mg+Fe^{2+})$$

$$Fe3\# \quad = \quad 100Fe^{3+}/(Fe^{2+}+Fe^{3+})$$

$$Ca" \quad = \quad 100Ca/(Ca+Mg+Fe^{2+})$$

$$Mg" \quad = \quad 100Mg/(Ca+Mg+Fe^{2+})$$

$$Fe" \quad = \quad 100Fe^{2+}/(Ca+Mg+Fe^{2+})$$

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

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

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).

Mineral 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 and Fe^{3+}.

For the reduced spinel prism the following components are calculated.

Mineral 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	ZnAl204	MgAl204	FeAl204
MnAl204	Mg2Ti04	Mn2Ti04	Fe2Ti04	MgCr204	FeCr204	MnCr204
Fe304						

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. An option allows calculation of ferric iron assuming 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).

Mineral names are:

P205	Zr02	Si02	Ti02	Al203	Cr203	V203
Y203	Fe203	FeO	MnO	NiO	MgO	CaO
Na20	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.PLT 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 metapath & preceeding characters in name

18 = Store plot parameters (on file)

Option [1 - 17] (Exit):

An example of a plot parameters file is given on pages 21-22 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 19 fonts, 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 are slightly different from those used by
the plotter (they are defined in the graphics package).

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 PLOT). The default symbol and text sizes are appropriate if the full page is used for 1 or more plots (see under PLOT), but may need changing if this is not the case. The numbers of axis labels and ticks on each axis are set automatically and cannot be selected by the user. However, the numbers will be reduced if plots are stacked or reduced in size. It is possible to set the tick size to zero, and add the required number of ticks by hand.

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.PLT);

A: (or A:\) would write the metafile to floppy disk drive A (e.g., A:GDA1PLT);

AB would add AB to the metafile name (e.g., ABGDA1.PLT);

D:\GDB\AB would write the metafile to directory GDB on drive D and add the prefix AB
(e.g., D:\GDB\ABGDA1.PLT).

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 selected for display)

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

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

10 — Define pen for mean lines (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:

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

2. Pen number.

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

4. Text (e.g., sample number or a legend; 0 - 50 characters).

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

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

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

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

    1. Single element (for selected groups)

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

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

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

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

    2. Pen number

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

    4. Text (e.g., a legend; 0 - 50 characters)

    5. Y-axis dataset (this specifies the dataset selected for a single

histogram (actually the X-axis in this case), or for any dataset
on a stacked plot of datasets)

<u>or</u>

Group number (this specifies the group for a stacked plot of
groups for one dataset)

Note: the given XY co-ordinates define the <u>centre</u> of the symbol or, if
no symbol is specified, the <u>bottom</u> 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
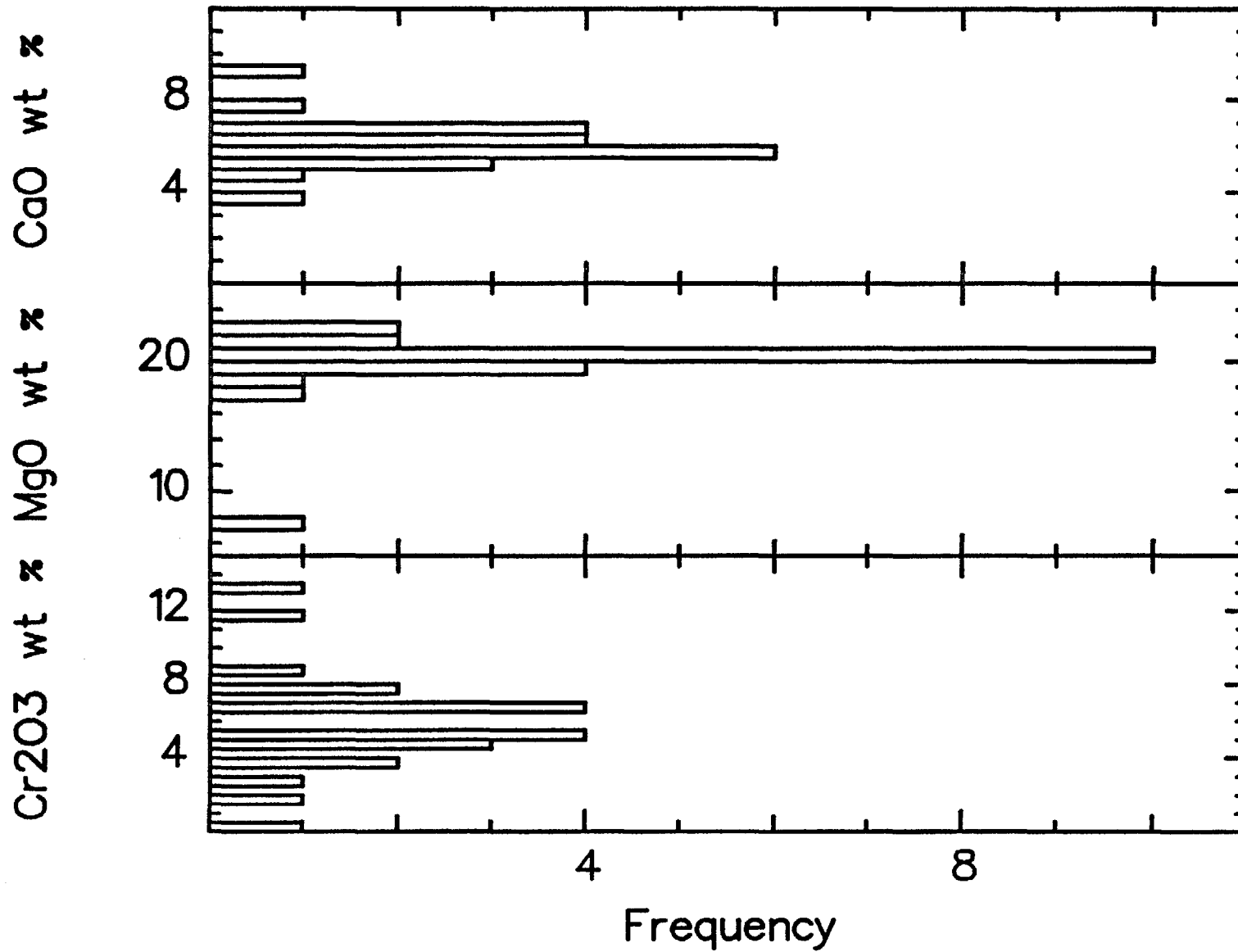
6.12 Display XY Plot

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

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

2. Pen number

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

4. Text (e.g., sample number or a legend; 0 - 50 characters)

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

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

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

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

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
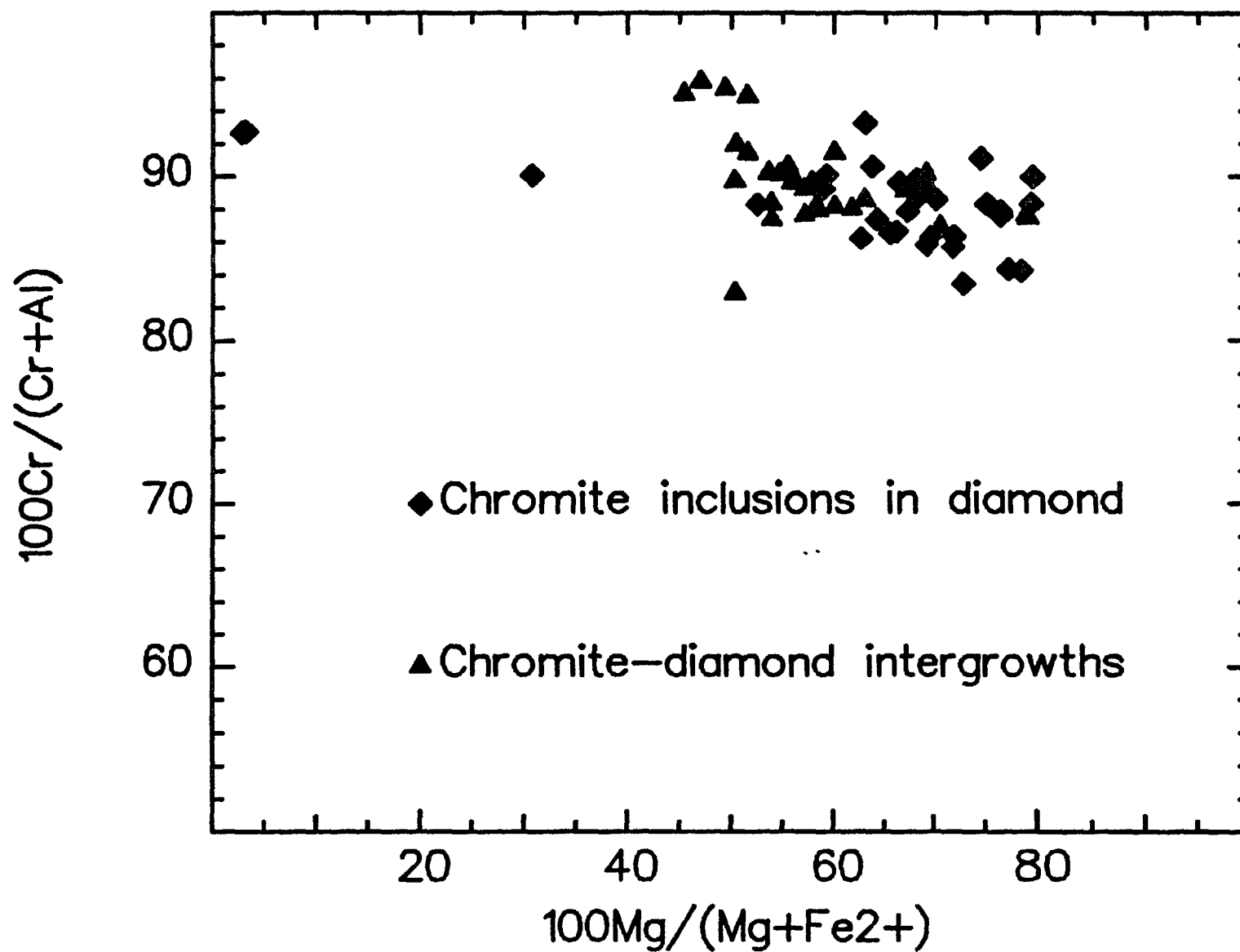
6.13 Display Triangular Plot

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:

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

      2. Pen number

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

      4. Text (e.g., sample number or a legend; 0 - 50 characters)

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

8   -   Specify graphics overlay files (xxx.GRF)

An example of an XYZ 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

MgO wt %

CaO wt %

Cr2O3 wt %

● Pipe M89 garnets

★ Pipe M97 garnets
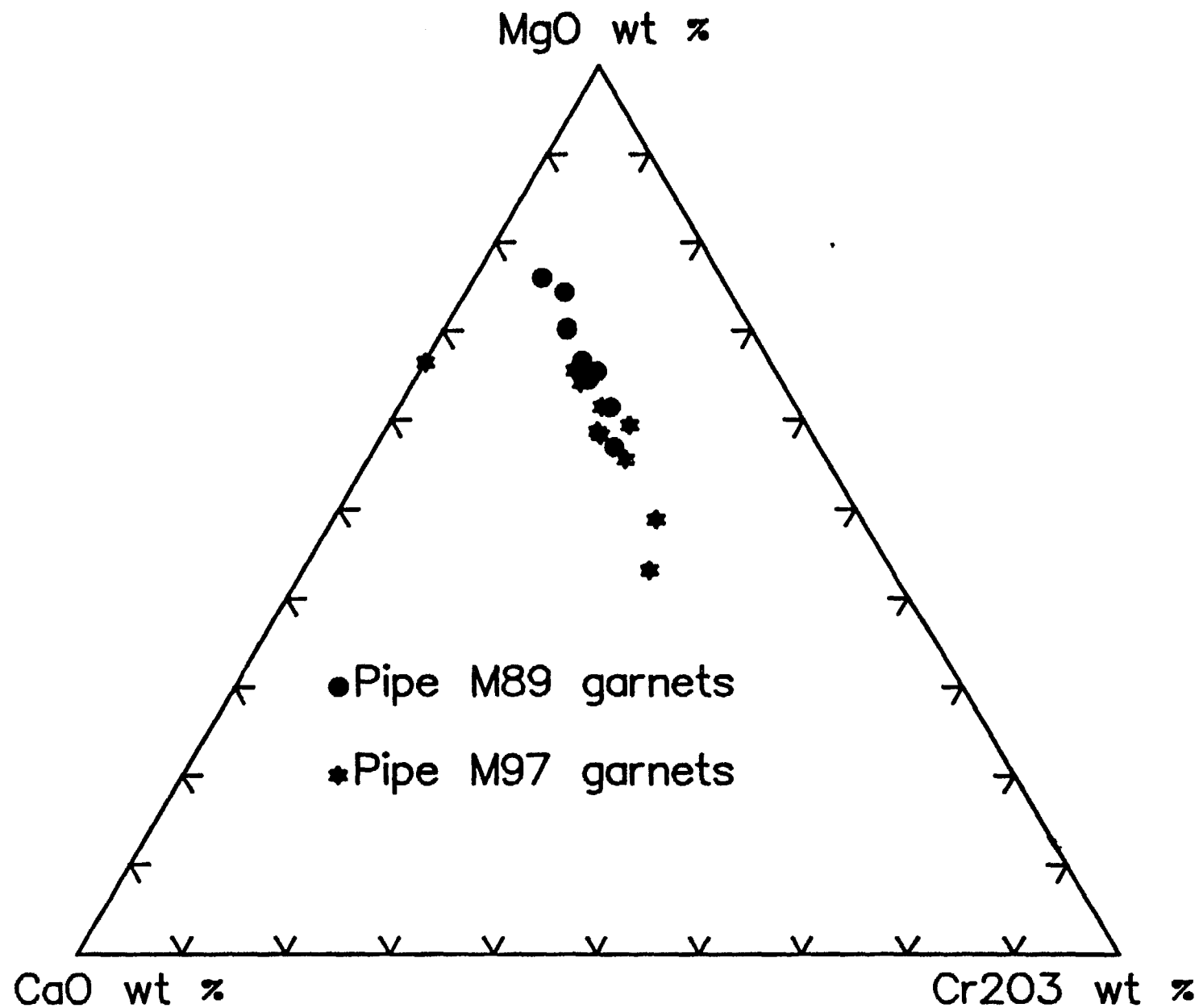
6.14 Display Legend

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 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

Example of the spinel prism plots for both the oxidising and reduced prisms is shown in Figures 4a,b.

FIG. 4A. OXIDISED SPINEL PRISM PLOT
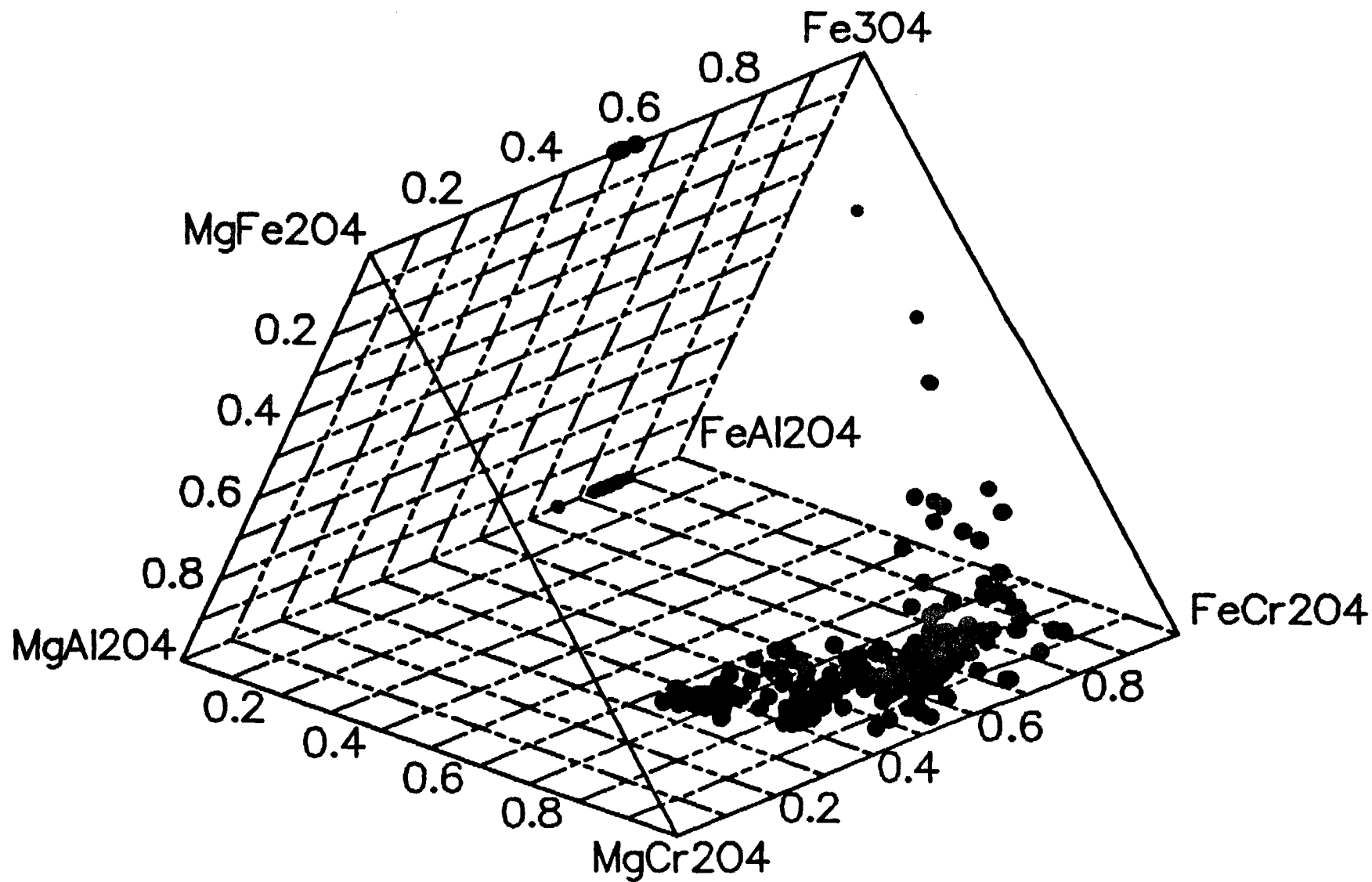
FIG. 4B. REDUCED SPINEL PRISM PLOT
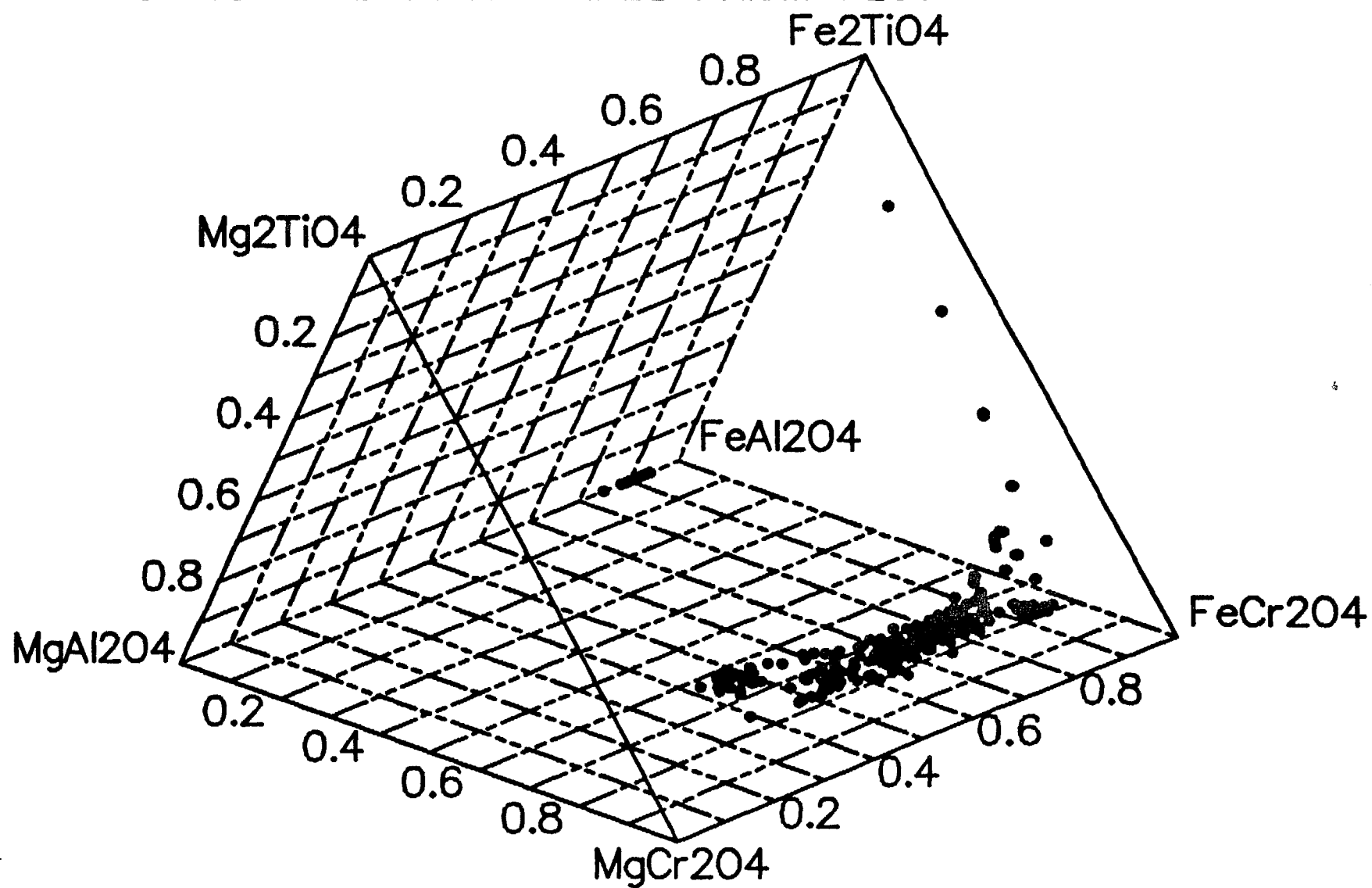
6.16. Box-Whisker Plot

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; fault 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 inclusion in diamond is shown in Fig. 5.

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

Weight percent

30.0

10.0

3.0

1.0

0.3

0.1

TiO2*10   Cr2O3   FeO   NiO*10   ZnO*10
      Al2O3   V2O3*10   MnO*10   MgO
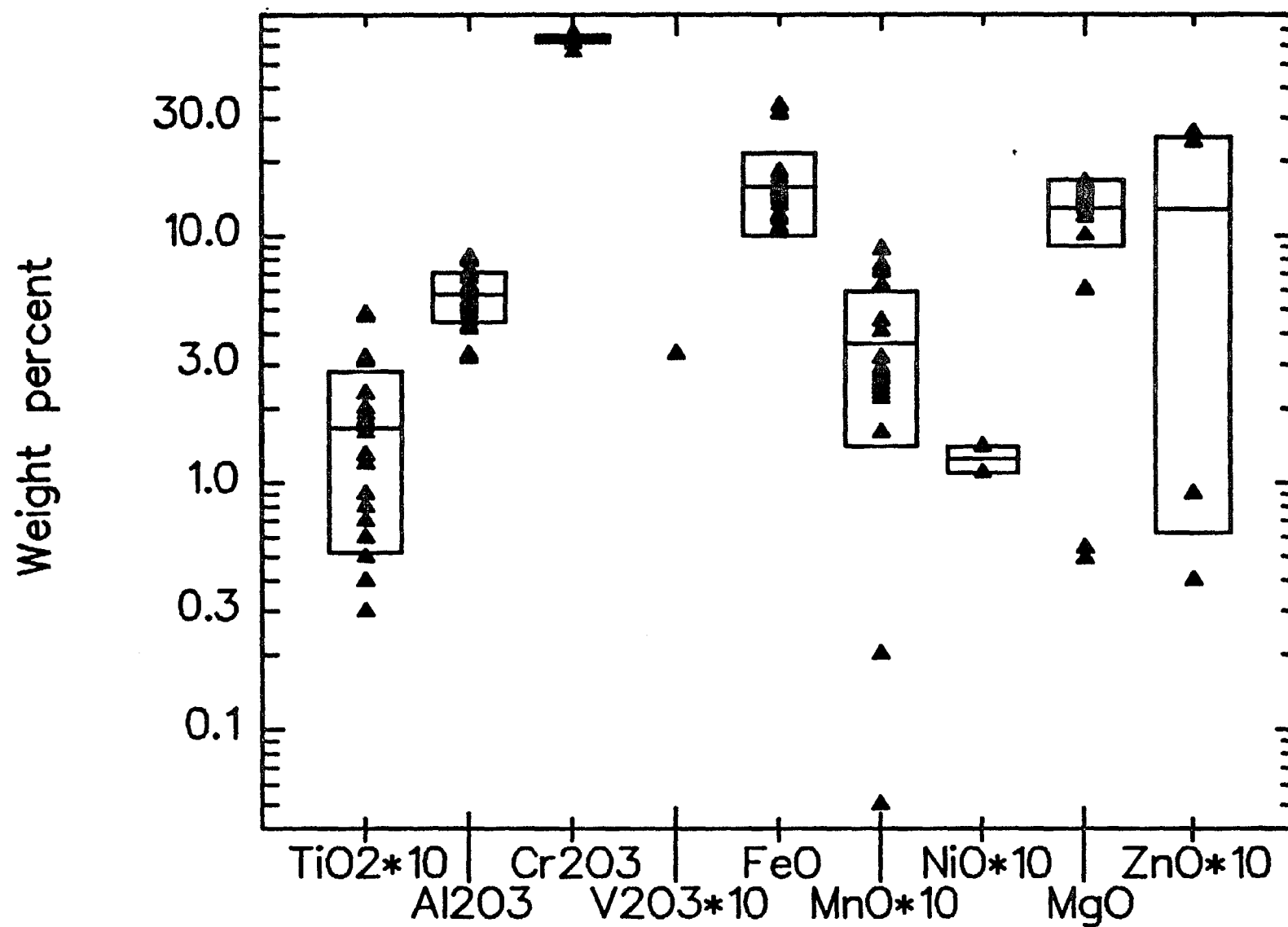
6.17. Print Structural formulae Report

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 a non-zero value value is held in the cations field. 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
A12O3	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.

	A	B	C	D	E
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 reports warnings if the number of oxygens in the formula sums to less than 6 or if any of the following rejection criteria apply:

a) $Si > 2.02$ or < 1.98

b) $ACF2T - Ti + Mg + Fe^{2+} + Fe^{3+} + Mn + Ni < 0.98$, where

   $ACF2T = Al^{M1} + Cr + Fe^{3+} + 2Ti$

c)   Sum of M2 cations < 0.98 or > 1.02

d) $ACF2T - Ca - Na - K - Al^{iv} > 0.030$

e) $Na > ACF2T$

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), $CaFe_2^{3+}SiO_6$ (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/enhanced by text editor 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 base end members in mol percent and the site allocation. It also provides an estimate of Fe_2O_3 content for microprobe analyses by normalisation of the the cations to either

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

or

b) 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 (in press). 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

1) Si + Al < 8.00

2) Si > 8.00

3) M1 cations > 5.00 i.e. $Cr + Al^{vi} + Fe^{3+}M1 + Ti > 5.00$

4) Ca > 2.00

5) M4 site cation deficient

6) Ca required in A-site

7) A-site cations > 1.00.

An exampe 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 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).

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, $MgCr_2O_4$, $FeCr_2O_4$, $MnCr_2O_4$ 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. The print file MDA.PRN may be printed direct or modified and enhanced by word processor.

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

	1	2	3
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

	1	2	3
O=	23.00	23.00	23.00

IMA(1978) CLASSIFICATION PARAMETERS

	1	2	3
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:
P205 (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

TABLE 6. EXAMPLE OF SPINEL REPORT

SPINELS REPORT - splherz.GDA

Analysis 75210425A2/1			SPINEL
	Wt %	O= 4.0	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 Reports

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/enhanced 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. PLOT

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

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

The PLOT menu, which is generated by typing PLOT or selecting option 5 on the combined GDA-MDA menu, is:

Output Metafile to connected plotter

```
1  -  Select plot (metafile)                    (  1)
2  -  Select speed of connected plotter         ( 10)
3  -  Select rotation for connected plotter     (  0)
4  -  Define number of plots/page               (  1)
```

5   -   Define plotting area within page   (.00 1.00   .00 1.00)

6   -   Switch output of plots to HPGL on a file

7   -   Output selected plot

8   -   Output all plots starting at selected one

9   -   Delete all metafiles (plots)

10 -   Delete all HPGL files

11 -   Define metafile path

12 -   Define HPGL file path

Q   -   Quit

Option [1.12,Q]:

Options 1-10 of the PLOT menu are dealt with on pages 54-71 of the GDA manual and are not repeated here. Examples of mineral plots generated under the MDAPROG and output to Laser printer from HPGL files are given in Figures 1-7.

Two additional options (11 and 12) allow different plot metafile or HPGL file paths to be specified.

(11)   Define metafile path (allows plot metafiles from a different disk drive or directory to be output to a connected plotter or as HPGL files).

(12)   Define HPGL file path (allows plot metafiles to be output as HPGL files on a different drive or directory).

In either case, the specified path is added to the beginning of the plotfile name (see examples under GDA, above). Due to line-length limitations of MS-DOS commands it may not be possible to specify complex pathnames for both metafiles and HPGL files simultaneously. Note that deleting metafiles and HPGL files (menu items 9 and 10) will only apply to those in the current (i.e. GDA) directory and only those without prefixes (e.g., GDA1.PLT, but not ABGDA1.PLT).

8. PRINT A TABLE OF MINERAL ANALYSES (TABMIN)

Tables of mineral analyses, including cation proportions in the structural formula, can be generated by selecting 17 or the GDA-MDA menu or by directly calling the program TABMIN. The tables generated have a different format from that generated by option 17 of the MDA 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

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

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). 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 file MINREPT.RPT is employed to define output. This can be modified as required to include other fields. 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 submenu is as follows:

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

2 = Select major elements (all by default)

3 = Select trace elements (all by default)

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

5 = Specify group titles

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

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

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

9 = Drop samples (anomalous samples may be 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 data 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 <u>assigned</u> samples have zero values, the dataset is automatically dropped out.

In order to run the cluster analysis program a cluster analysis file must first be generated in the STATS program, which includes options to add arithmetic expressions, drop elements and samples, and select groups.

To run the program (which actually includes two parts, CLUSTA and DEND), type CLUSTER or option 7 of the GDA-MDA menu to generate the cluster analysis file.

A cluster analysis file (normally of the form ????.CLU) must be specified, followed by the options listed below:

1. Q-mode (default) or R-mode.
2. The similarity measure-correlation coefficient (default) or proportional similarity coefficient.
3. The linkage method - weighted-pair group method (default) or unweighted.
4. Highest value of similarity (i.e., the upper limit of the Y-axis: 0-1, 1.0 by default).
5. Lowest value of similarity (i.e., the lower limit of the Y-axis: 0-1, 0.0 by default).

Note that the calculations take a significant amount of time to carry out. 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 are given in Tables 10 and 11 of Q-mode and R-mode cluster analysis for a suite of garnets from the Wandagee alkaline intrusives.

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

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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. DEND (DENDOGRAMS FOR CLUSTER ANALYSIS)

Dendograms of the cluster analysis generated by program CLUSTA may be
displayed using program DEND which is invoked by typing DEND or option 8 of
the GDA-MDA menu. The dendograms may be displayed on screen or output to a
metafile (GDA1.PLT to GDA99.PLT). The metafiles may be output to either a
directly-connected HP or HP-compatible plotter or converted to HPGL files for
use on off-line plotters and laser printer using the PLOT 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 Figs 6A and 6B.

Fig. 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.

Fig 6B is an example of R-mode cluster analysis using the proportional
similarity coefficient.
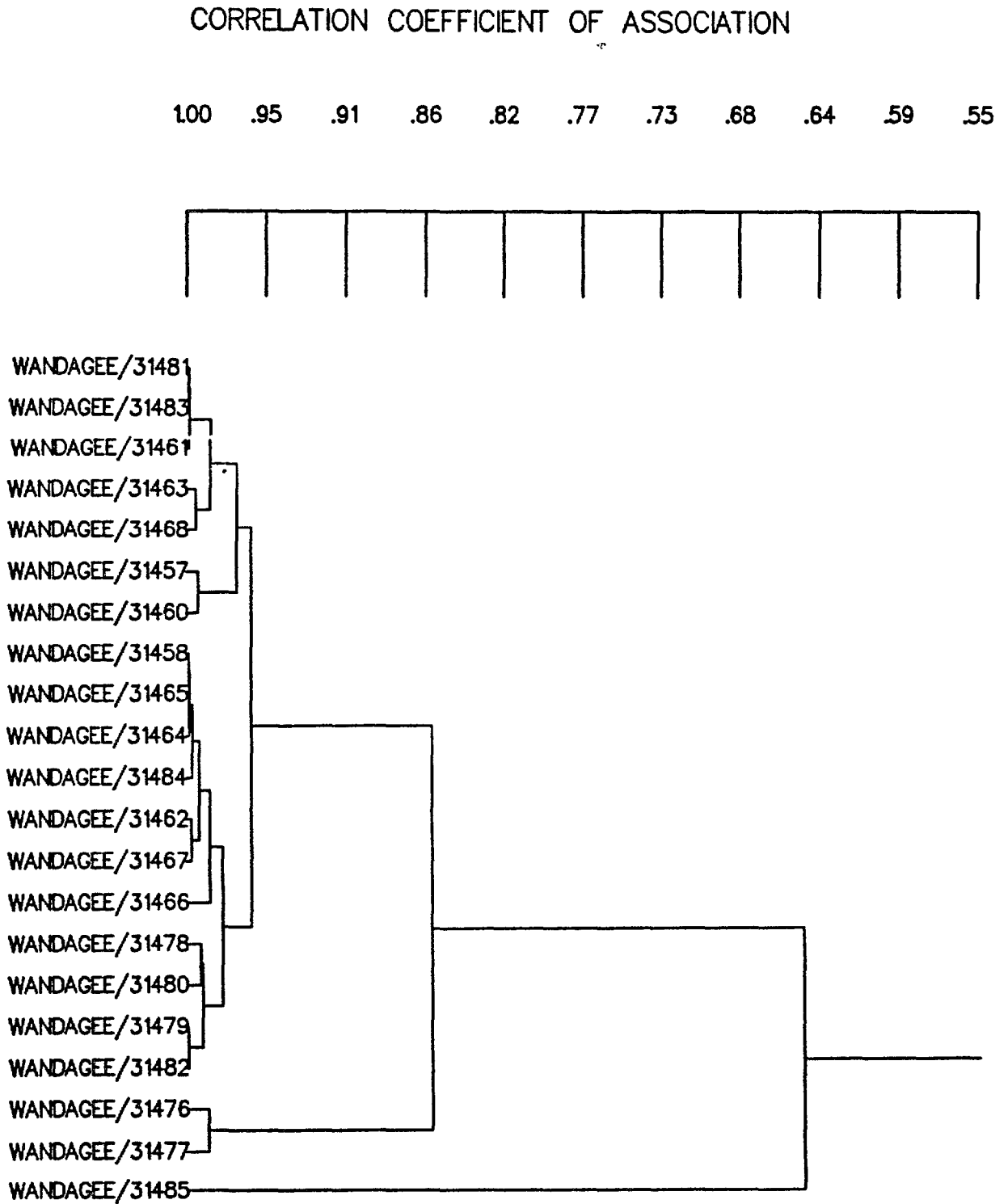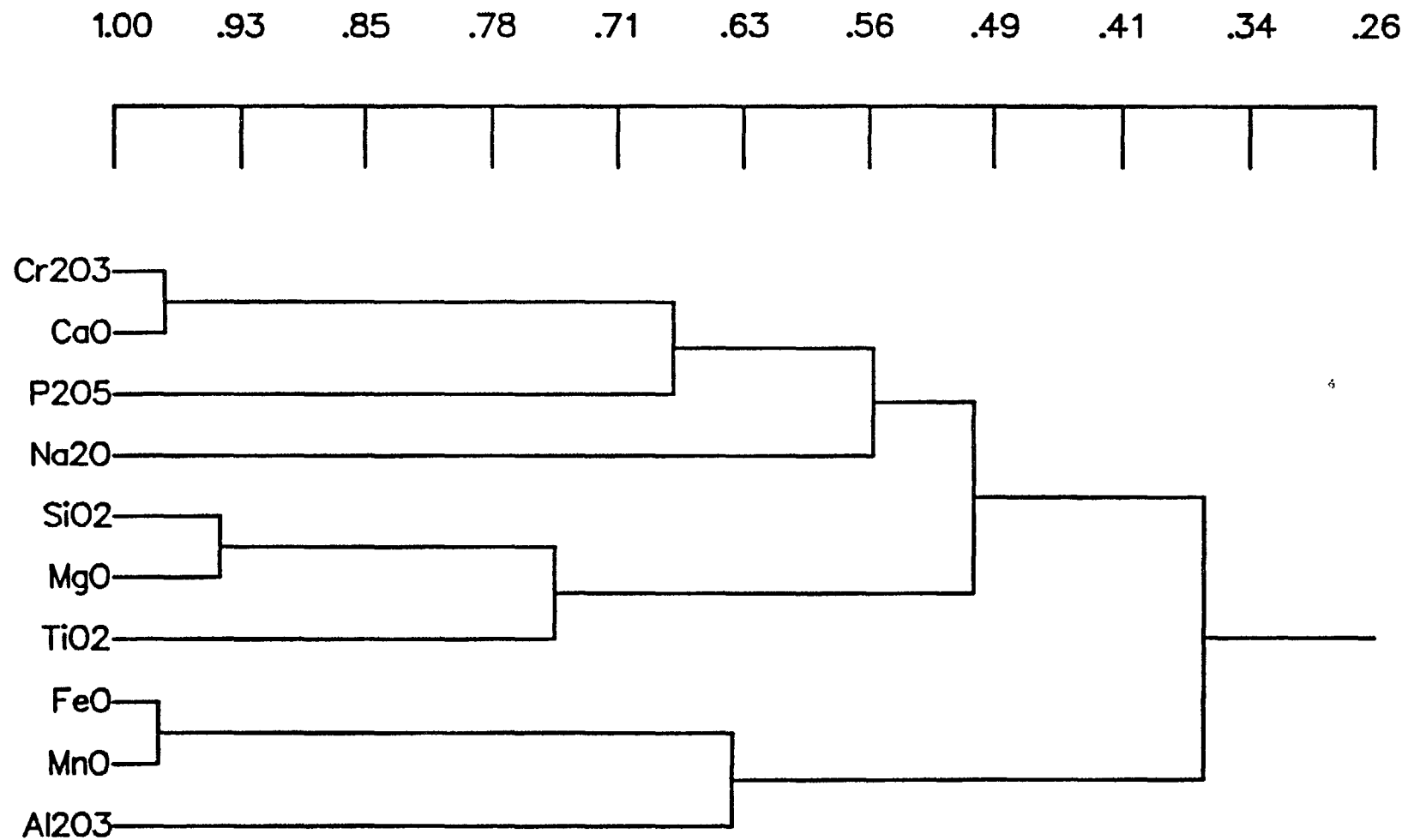
FIG. 6A. Q—MODE DENDOGRAM OF GARNET COMPOSITIONS

CORRELATION COEFFICIENT OF ASSOCIATION

| 1.00 | .95 | .91 | .86 | .82 | .77 | .73 | .68 | .64 | .59 | .55 |

WANDAGEE/31481
WANDAGEE/31483
WANDAGEE/31461
WANDAGEE/31463
WANDAGEE/31468
WANDAGEE/31457
WANDAGEE/31460
WANDAGEE/31458
WANDAGEE/31465
WANDAGEE/31464
WANDAGEE/31484
WANDAGEE/31462
WANDAGEE/31467
WANDAGEE/31466
WANDAGEE/31478
WANDAGEE/31480
WANDAGEE/31479
WANDAGEE/31482
WANDAGEE/31476
WANDAGEE/31477
WANDAGEE/31485

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 on the 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)

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; 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 groups 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.

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 locality, lithology, or
   age. Samples in a group are plotted with the same symbol and colour. It
   is recommended that the logic is stored on a file for subsequent re-use
   and/or editing.

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

4. The main minerals analysis program (MDAPROG) contains 23 application
   programs which enable generation of plots, initially on the PC screen, and
   then as plot metafiles for output to plotters, and preparation of tables of
   anlayses. 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 then used to
   produce histograms, XY plots, triangular plots, and box-whisker plots. The

required plots are then written to metafiles for subsequent output to plotters. 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 prism. MDAPROG also has the facility to generate tables of mineral analyses, structural formulae and derived arithmetic ratios.

5. Output of plot metafiles to plotters is carried out by the PLOT program. Plots may either be output directly from metafiles to a connected plotter, or written to HPGL files for output to an offline plotter or laser printer. There are facilities for positioning plots on a page, and for outputting a number of plots on a single page.

6. 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

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APPENDICES

A. SYSTEM LIMITATIONS

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

Max	Description
50	number of groups
11	number of datasets (GDAPROG)
50	number of datasets (SMALLGDA)
4	number of datasets (BIGGDA, MDAPROG)
800	number of assigned samples (GDAPROG)
400	number of assigned samples (MDAPROG)
200	number of assigned samples (SMALLGDA)
2000	number of assigned samples (BIGGDA)
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
5	number of additional points for plots
10	number of columns in report
800	number of samples for least squares line fit (GDAPROG)
200	number of samples for least squares line fit (SMALLGDA)
0	number of samples for least squares line fit (BIGGDA, MDA)

15   number of minerals for modelling

10   number of least squares mixing minerals

12   number of olivine addition oxides

5000 number of samples in a GDA file that can be sorted or merged by the UTIL

program

250   number of samples or variables in CLUSTER program

50   number of characters of text for added plot points or text

20   number of additional plot points and/or text lines.

B. SOFTWARE MAINTENANCE

Most software files are held on directory\GDA\ with the HALO system on \HALO\. The directory\BIGGDA\ is used for building the larger capacity GDA program BIGGDA,\SMALLGDA\ is used for the small capacity GDA program SMALLGDA, and\MINGDA\ for the minerals program MDAPROG.

The programs use software simulation of floating point operations so they will run on most PCs. The software is written in FORTRAN 77 (Microsoft compiler) and consists of some 60 programs and over 20 000 lines of source code occupying approximately 1Mb of disk space. The exception is the arithmetic calculator routine ARITH.IFT, which is written in a higher level language IFTRAN. This code must be run through the IFT preprocessor to produce the FORTRAN source code. If the system is transported to another computer the FORTRAN source ARITH.FOR can be used directly, although it is not very readable. There has not been enough time to convert the routine to standard FORTRAN.

The insert files for the required directories (GDA, BIGGDA, SMALLGDA, MINGDA) should be copied into \GDA\.

The whole system can be built by typing 'all' in directory\GDA\. This will direct the correct files to be copied to the appropriate directory, compiled and linked.

Each program has a file (with extension .LNK) that is used for linking. Some programs have a simple overlay structure. All COMMON blocks and major arrays are on files (with extension .INS) and are inserted by the compiler into the source code.

Changing a system limit requires modifying array definitions in the insert files, changing the limit definition in GDABLK.FOR and typing 'all' to rebuild. The separate directories \BIGGDA\and\SMALLGDA\ hold a second set of definitions for the version of the program that allows different numbers of samples to be handled, and a version of GDABLK.FOR that defines the limits. Similarly, the \MINGDA\ directory has insert files for the MDAPROG program.

The least squares line fitting has been dropped from BIGGDA and MDA because of memory limitations imposed by DOS.

The source code (FORTRAN) files (on each directory) can be backed up to floppy disks with the command file BACKUP. Only one (1) copy is permitted under copyright.

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

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

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

1. Install Microsoft FORTRAN.
2. Create HALO, GDA, BIGGDA, SMALLGDA and MINGDA directories.
3. Copy the HALO files for Microsoft FORTRAN to \HALO\.
4. Copy from \HALO\ into \GDA\;
   - The appropriate plotter translator file(s) which should be renamed, e.g., copy halo HALO7550.EXE HP7550.EXE,
   - All *.FNT files (fonts),

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

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

5. Copy the source floppies to \GDA\.

6. Type 'all' under GDA.

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

C. 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.

The GDA manual (pages 133-148) gives examples of the various parameter files used in extracting data in the GDA program. The main parameter files used for MDA are:

OXIDE.DEF   - contains the element to oxide conversion factors for most of the periodic table. This is used for analyses of silicates and oxides.

METAL.DEF   - similar to OXIDE.DEF but used for analyses of metals and sulphides.

OXIDE.MTB)   - report definition files used in MDAPROG.
METAL.MTB)

MINREPT.RPT   - Report definition file containing some 23 common major elements as oxides to be used in generating reports of analyses of oxides using TABMIN.

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 (see also pages 133-134 of the GDA Manual). OXIDE.DEF, OXIDE.MTB and MINREPT.RPT are given in the following pages.

PARAMETER FILE OXIDE.DEF

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

```
03    Li Li20        1.47304
04    Be BeO         2.77530
05    B  B203         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 Na20        1.34797
12    Mg MgO         1.65807
13    Al Al203       1.88946
14    Si SiO2        2.13932
15    P  P205         2.29137
16    S  SO3         2.49694
17    Cl Clwt        1.0
18    Ar Arwt        1.0
19    K  K20         1.20458
20    Ca CaO         1.39920
21    Sc Sc203       1.53384
22    Ti TiO2        1.66806
23    V  V203         1.47919
24    Cr Cr203       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 Ga203       1.34423
32    Ge GeO2        1.44083
33    As As203       1.32032
34    Se Sewt        1.0
35    Br Brwt        1.0
36    Kr Krwt        1.0
37    Rb Rb20        1.09360
38    Sr SrO         1.18261
39    Y  Y203         1.26994
40    Zr ZrO2        1.35080
41    Nb Nb205       1.43053
42    Mo MoO3        1.50031
44    Ru Ruwt        1.0
45    Rh Rhwt        1.0
46    Pd Pdwt        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 Cs203       1.06019
56    Ba BaO         1.11648
57    La La203       1.17277
58    Ce Ce203       1.17128
59    Pr Pr203       1.17032
```

```
60      Nd Nd203        1.16639
62      Sm Sm203        1.15962
63      Eu Eu203        1.15793
64      Gd Gd203        1.15262
65      Tb Tb203        1.15101
66      Dy Dy203        1.14770
67      Ho Ho203        1.14551
68      Er Er203        1.14349
69      Tm Tm203        1.14206
70      Yb Yb203        1.13869
71      Lu Lu203        1.13716
72      Hf Hf203        1.17929
73      Ta Ta205        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  U308         1.17925
```

PARAMETER FILE MINERAL.MTB

Report definiton file MINERAL.MTB
Major elements
62
U308
MoO3
P205
Nb205
Ta205
SiO2
ToO2
GeO2
ZrO2
WO2
ThO2
B203
Al203
Sc203
V203
Cr203
Ga203
As203
Y203
Cs203
La203
Ce203
Pr203
Nd203
Sm203
Eu203
Gd203
Tb203
Dy203
Ho203
Er203

Tm_2O_3
Yb_2O_3
Lu_2O_3
Hf_2O_3
Fe_2O_3
FeO
MnO
NiO
MgO
CoO
CuO
ZnO
CaO
SrO
BaO
PbO
Li_2O
Na_2O
K_2O
Rb_2O
O
F
Ne
Cl
Ar
Br
Kr
I
Xe
CO_2
NO_3
Trace elements
62
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
H

```
Er
Tm
Yb
Lu
Hf
Fe
Fe3+
Fe2
Mn
Ni
Mg
C
Cu
Zn
Ca
Sr
Ba
Pb
Li
Na
K
Rb
F
Ne
Cl
Ar
Br
Kr
I
Xe
C
N
Description fields
7
SAMPNO        Sample number
ANALNO        Analysis number
MINERAL       Mineral name
MINDERSCR     Description
STRATGROUP    Stratigraphic Group
STRATUNIT     Stratigraphic unit
STRATHT       Stratigraphic height
```

PARAMETER FILE MINREPT.RPT

```
Report definition file MINREPT.RPT
Major Elements
23
P205        P205
NB205       Nb205
ZR02        Zr02
SI02        Si02
TI02        Ti02
AL203       AL203
CR203       Cr203
V203        V203
Y203        Y203
FE203       Fe203
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
6
ANALNO      Analysis number
SAMPNO      Sample number
MINERAL     Mineral
MINDESCR    Mineral description
OXYGENS     Number of Oxygen atoms
CATIONS     Number of cations
```

D. GRAPHICS OVERLAY FILES

Graphics overlay files are used to add extra information, such as text and field boundaries, to XY and triangular plots. In particular, field boundaries used in various 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. If the axes limits selected for XY plots are less than those covered by the overlay file, lines will be truncated on the screen, but not necessarily on the paper plots due to limitations of HALO.

An example of a graphics overlay file used to discriminate mantle garnets on a wt Cr_2O_3 versus CaO diagram (Sobolev et al, 1973) is given below and its application shows in Figure 7. Further examples of graphics overlay files are given in pages 151-183 of 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
```
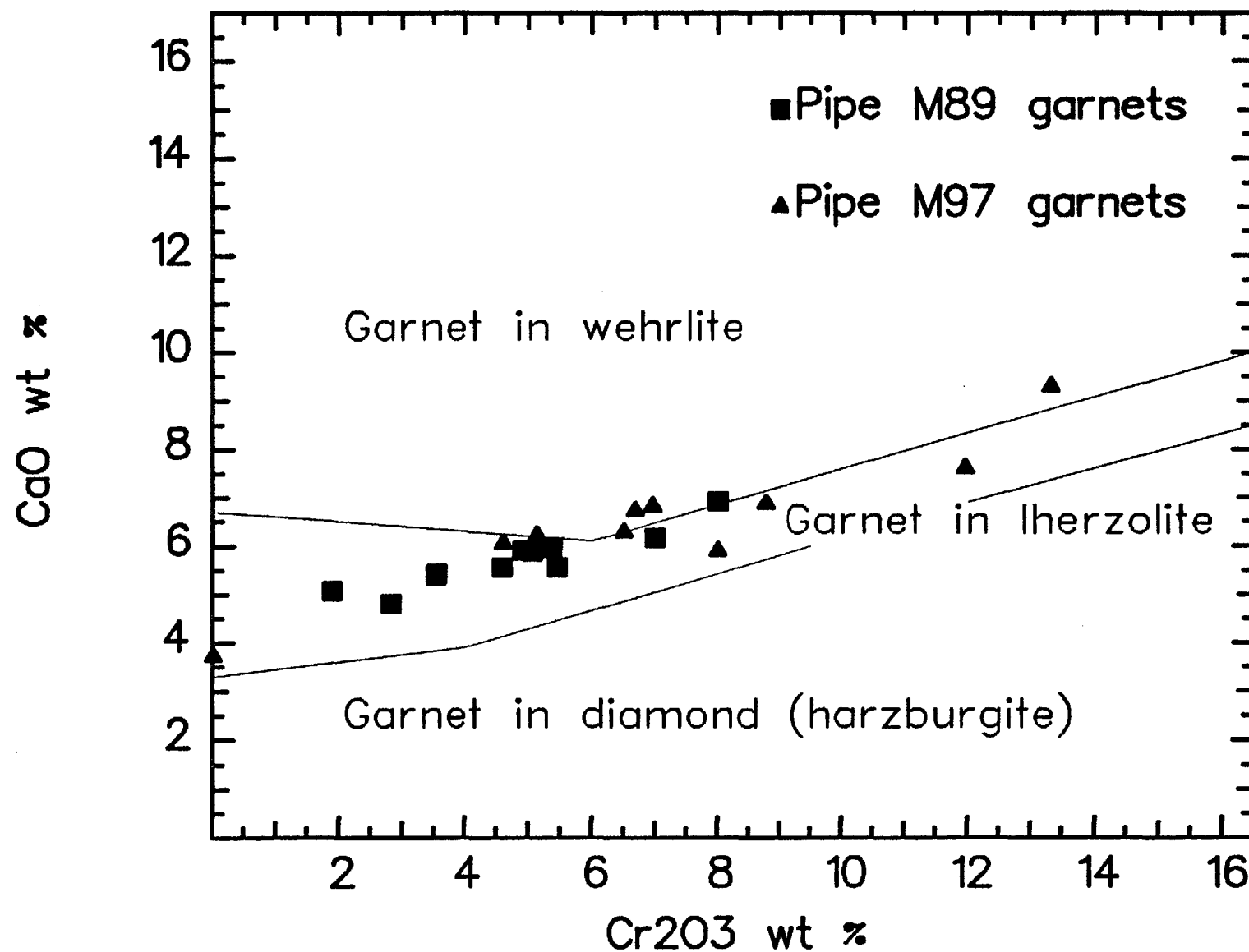
6.0,6.1

Line   2

6.0,6.1

16.5,10.0

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

E. TRANSFER OF DATA FROM ANU/BMR ELECTRON PROBE MICROANALYSER

Data are transferred from the ANU/BMR Cameca (Camebax) EPMA to ASCII files on
an IBM PC floppy disk using the program PROCOMM. The data can then be read
into the GDA/MDA system using program PROBE. To transfer analyses from the
Dec PDP 11 controlling the Cameca to the IBM PC at the probe the following
instructions apply.

1. Turn on PC (PC should be in the MCA directory);

2. Type CD\PROCOMM followed by GO when in PROCOMM directory
   (This will instal the PROCOMM program used to transfer the data);

3. Insert floppy disk into Drive B;

4. Press F10 (for help Menu);

5. Selection 'ASCII Receive' option by pressing F6;

6. Enter file name specifying the B drive i.e. B:filename;

7. On PDP 11 exit to operating system;

8. Type R PCFILE (return);

9. Respond to 'Enter header line' request by entering header;

10. Respond to 'Enter lower analysis number (1 to 1000 for current file)'
    by entering the lowermost analysis number;

11. Respond to 'Enter upper analysis number (1 to 1000 for current file)'
    by entering the uppermost analysis number;

12. Respond to 'Analyses for deletion (1 to 1000 current file)' by
    entering up to 20 analyses to be deleted. Enter 0 for no deletions;

13. Repeat for subsequent groups and enter 0 for lower analysis number to
    end;
    This process generates file IBMPC.TXT (IBMPC.TXT; 1, 2, etc, for
    several files);

14. Type COPY IBMPC.TXT.TT3: [Note: Do not hit return key until PROCOMM is
    ready to receive the file - see 1-6];

15. Hit RETURN/ENTER key on PDP 11 keyboard to commence transfer;

16. On completion of transfer of data, press ESC to exit;

17. Exit from PROMM (ALT X COMMAND);

18. Check floppy disk for correct transfer of data.

The data is entered into the MDA/GDA system via program PROBE. Program PROBE requires the name of the data file and the new Oracle (.ORC) file. The program then scans the data file for the listed elements and reports any errors/corrupted data. Descriptive information - sample number (SAMPNO), mineral (MINERAL), mineral description (MINDESC), the number of oxygens (OXYGENS), and, if required, the number of cations in the ideal formula (CATIONS) to enable calculation of Fe_2O_3 and FeO based on stoichiometry - are then entered. Incorrect entries can be corrected interactively and poor analyses can be rejected from the Oracle file. The program stops when it reacheas the end of file character 99 in the element listing.

NOTE: If it is necessary to exit from PROBE and resume later a new .ORC file must be nominated to avoid overwriting the original file used in the previous session, i.e., program PROBE does not allow appending of files.