GEOLOGICAL SURVEY OF CANADA

OPEN FILE 2596

MINREP
A FORTRAN computer program to produce tables of mineral analyses with formulae and end members

G.J. Pringle

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Natural Resources Canada Ressources naturelles Canada

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MINREP

A FORTRAN Computer Program to Produce Tables of Mineral Analyses with Formulae and End Members

G.J. Pringle
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ABSTRACT

MINREP is an interactive DOS based FORTRAN program designed to produce formatted tables of mineral analyses that include formulae, molecular end member values and molecular ratios. The user may quickly choose or alter the details of the format of the table that is to be printed. This includes the list of up to 20 chemical elements or oxides, their order, the formula basis, the formula sites, the elements in each site, the distribution of elements between sites, the basis of calculated Fe^{+3} and Fe^{+2}, the definition of up to 20 end members and up to 20 cation ratios. Data may be edited, restructured and averaged. The data is imported as ASCII text and the tables of restructured data may be printed directly or written to ASCII text files which in turn may be passed to a variety of word processing or spreadsheet packages. The program is provided on DOS compatible diskette accompanied with a printed installation and users guide.

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INTRODUCTION

The microprobe laboratory at the Geological Survey of Canada has been involved in producing microbeam analyses of minerals for over 30 years. The newer instrumentation produces a great volume of data which in turn presents particular problems with the collation of results and the preparation of tables summarizing the results. This is particularly true when mineral formula calculations are required.

In 1989 we developed an on-line analytical program for the energy-dispersive spectrometers that included an extensive mineral formula calculation option (EDDI GSC Open File 2127, 1989). This portion of the older program has been expanded and transported to an DOS compatible system where it forms the basis of the program MINREP which is in routine use at the GSC.

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PROGRAM INSTALLATION

a) Hardware and memory requirements

DOS compatible environment with 330 Kb of free memory.

High density 3 1/2" disk drive.

DOS compatible printer.

Minimum of 4 Mb free space on the hard drive.

b) Installation

Check that your hard drive has enough free space.

Create a sub-directory on the hard drive. (eg. C:\MR)

Copy MREPORT1.EXE from the distribution diskette to the new sub-directory on the hard drive. This file is a self extracting compressed archive.

Change the default directory to the new sub-directory. (eg. C:\MR)

Extract and decompress the program files by running MREPORTS.EXE

The directory C:\MR should be as follows -

```
AMPHIBOL.DAT     2233  06/30/95 11:59 |  ANDIDOCU.       4000  06/30/95 11:59
ANDIGSC1.        4000  06/30/95 11:59 |  ARROW   .WPG     206  06/30/95 11:59
ATNO    .         184  06/30/95 11:59 |  ATWT    .        368  06/30/95 11:59
CMMT    .TXT      122  06/30/95 11:59 |  CONVTAB .EXE   45878  06/30/95 11:59
DUMP    .        3733  06/30/95 11:59 |  FODIDOCU.       1600  06/30/95 11:59
FODIGSC1.        1600  06/30/95 11:59 |  MANUAL  .WPD  322855  06/30/95 11:59
MR      .EXE   328138  06/30/95 11:59 |  MREPORT1.EXE  317644  06/30/95 11:59
MREPORTS.TXT     4494  06/30/95 11:59 |  PRNCOD  .        640  06/30/95 11:59
SANADOCU.       75000  06/30/95 11:59 |  SANAGSC1.       75000  06/30/95 11:59
SFORDOCU.     1600000  06/30/95 11:59 |  SFORGSC1.     1600000  06/30/95 11:59
VALE    .         184  06/30/95 11:59 |
```

Appendix A gives more details on what is contained in each of these files and their relationship to the operation of the program. MREPORTS.EXE may be deleted.

c) Running the program

Change directory to C:\MR

Type - MR [Enter]

The program displays its command menu after you have toggled past the title page. Commands are entered by menu number at the asterisk (*) prompt.

d) Printer configuration

The program has a selection of two default printer configurations. On installation it is set for a Roland[DG] PR-1215 dot matrix printer and should work well with any standard dot matrix printer. The printer configuration option in the utility sub-menu may be used to switch to the other default set-up which is for a HP LASERJET IIP.

The printer configuration option in the utility sub-menu may also be used to alter these default printer configurations if there are inconsistencies with your printer. The printer configuration consists of a series of parameters and printer control codes. The most likely change that will be useful is the page length. It is particularly important that the compressed print, the normal print and the reset codes are correct. Most printer manuals give the correct codes.

Selections made in the printer configuration option are permanently stored in the PRNCOD file, hence the changes only need to be made once.

e) Default valences

The disk file VALE contains default values for the valence of any element to be processed in the form of oxide components. These may be initialized or changed with a command in the utility sub-menu.

PROGRAM DESCRIPTION

1) STRUCTURE

The purpose is to be able to produce formatted tables of mineral analyses that include formulae, end member values and cation ratios.

The program is structured around the following command menu ...

```
                    MINERAL FORMULA UTILITY
                    ***********************

1) CHOOSE A FORMULA              11) ANALYSIS DIRECTORY
2) ENTER A NEW FORMULA           22) OUTPUT RESULTS
3) SAVE CURRENT FORMULA          33) ENTER WT.%
4) DELETE FORMULA                44) EDIT ANALYSES
5) DISPLAY CURRENT FORMULA       55) PRINT RAW DATA
6) CHANGE FORMULA BASIS          66) DELETE ANALYSES
7) SPECIFY END MEMBERS           77) LOAD FROM ASCII FILE
8) SPECIFY RATIOS                88) WRITE TO ASCII FILE
9) UTILITY OPTIONS               99) CHANGE FORMULA DIRECTORY
0) EXIT PROGRAM                  00) CHANGE ANALYSIS DIRECTORY

*
```

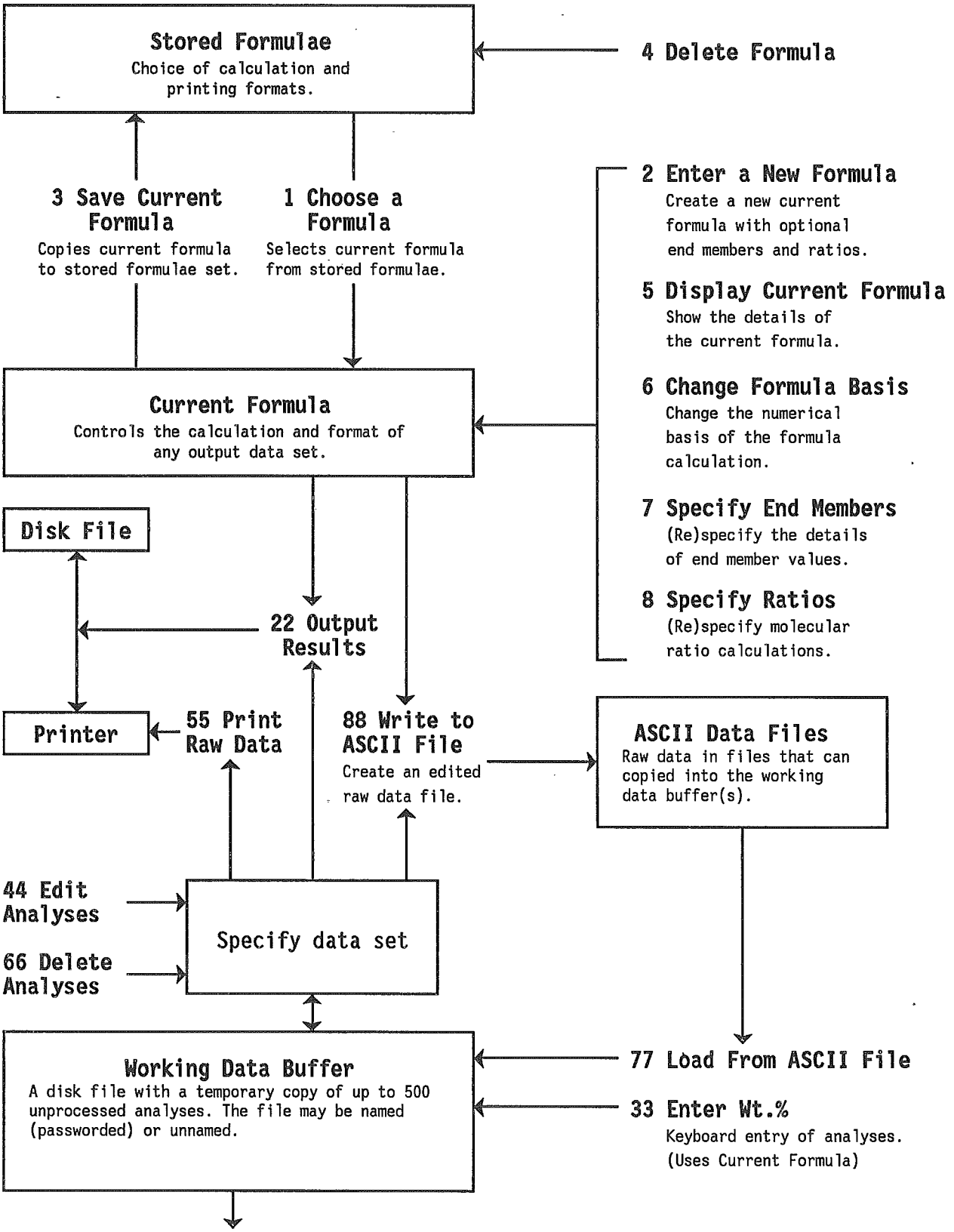
Figure 1 on the following page is a flow chart of the essential elements of the program architecture. These provide the key to the individual command descriptions in the following chapter.

The general steps in using the program are -

a) Load the original unprocessed analyses into a buffer.
b) Describe how the analyses are to be recalculated.
c) Describe the output format.
d) Specify which analyses are to be processed.
e) Send the output to the printer or to a disk file.

The **Working Data Buffer** is a disk file with a copy of up to 500 analyses in raw form. The program can import data into this buffer from an DOS (ie. ASCII) text file that has the correct format. This required format is simple to produce in all of the commonly used word processing, data base or spread-sheet packages. The details of the format are given in Appendix D.

Figure 1. PROGRAM OUTLINE



Often the most difficult step is capturing original analyses from the controlling computer of an analytical instrument, particularly if it is not DOS based. In our case we use a communications program and a simple linkage to a printer or serial port on the analytical instrument. Provision has also been made for keyboard entry of analyses into the working data buffer.

The working data buffer is a temporary storage file with a size limit. This can be a constraint when you are working with larger volumes of data or when a number of individuals are using the same copy of the program. To help with this problem, access is provided to multiple working data buffers by means of passwords. The working data buffer in the installation copy of the program with the password DOCU contains the compositions used as illustrations in this documentation (00) CHANGE ANALYSIS DIRECTORY).

The term **Formula** is used to encompass all the details of how the analyses are to be recalculated and what the format of the table is to be. This terminology arose because the initial keyboard entry of the format is in the form of a character string that is the same as a mineral formula written with bracket site delimiters and subscripts. Within this context a formula can include -

1) The elements in the analysis.

2) The order that the elements appear in the table.

3) Oxide or element format.

4) Valence of the oxides.

5) Fe as FeO or Fe_2O_3 or both.

6) Stoichiometric Fe^{+2} or Fe^{+3}.

7) The number of sites and cation total for the iron calculation.

8) Basis of normalization for the formula. This may be on total cations, cations in some sites, total oxygens, total oxygen and oxygen equivalents of negatively charged species or total anionic species.

9) Boundaries of formula sites in the element list.

10) Elements to be shared between sites. The elements are shared by defining an order of site filling.

11) Definitions of end member molecules to be calculated as mol % and/or weight % values.

12) Definitions of mol.% cation ratios to be used as plotting co-ordinates.

The **Current Formula** is the currently active selection of these parameters which may have been entered through the keyboard or selected from previously prepared formulae retained on the hard disk. The installation copy of the program has a selection of frequently used formulae in the default directory. The formulae used as illustrations in this documentation are in the directory with the password DOCU (99) CHANGE FORMULA DIRECTORY).

The process of entering a format through the keyboard, thereby creating an original current formula, can be simple or complex. This depends on the nature of the job at hand. Often the process is as simple as entering the mineral formula as a character string. However the program is not designed to teach the user how to calculate mineral formulae and end member molecules. Appendices B and C are an introduction to these calculations and you should become familiar with them before attempting to create a formula of any complexity within the program, particularly where end member calculations are concerned. As a learning exercise, you should try to duplicate some of the formulae included in the installation copy of the program. When you have created a new format, it is a good practice to cross-check what the program is doing with some hand calculations. End member calculations may be verified by processing a composition that is equal parts of the theoretical end member molecules. These steps will intercept errors and will help identify cases where the calculation that you expected exceeds the logic built into the program.

The set of analyses that are to be reported may be selected from the working data buffer in any order by their buffer sequence numbers or by indicating a wildcard label that is keyed to the eight character label that is stored with each analysis.

Output may be directed to the printer, to an ASCII disk file in table format or to an ASCII disk file in raw data format (Appendix D). Disk files in table format may be easily imported into a word processing program and then printed on a high quality printer. The disk files in raw data format are suitable for reloading into the working data buffer thereby providing a method of editing and restructuring the original data.

Disk files of results in table (column orientation) format are difficult to import into spreadsheets or databases. A separate utility program called CONVTAB has been provided to deal with this problem. It will convert tables produced by MR into row orientation. CONVTAB has instructions that are displayed at runtime.

2) YES/NO CONVENTION

The program is self prompting after any selection from the main menu. As you proceed you are presented with a series of requests for information, often in the form of a query that requires a (Y)es or (N)o answer.

If the query string is in the form - **Query? [x]:** - the bracketed item is the default response which may be accepted by an [Enter]. When the query string is in the form - **Query? [Y/N]:** - then the response must be Y[Enter] or N[Enter]. Any other character including [Enter] will repeat the query. This form is used in situations where an unintended response will cause difficulty.

3) ANALYSIS NUMBERING

The program distinguishes the analyses in the working data buffer by means of their sequence number in this file. This is the number given by the directory command in the main menu (11) ANALYSIS DIRECTORY). When you are processing a sub-set of data from the buffer the program will prompt you to enter a number string that identifies the data.

```
ENTER ANALYSIS NUMBERS
#?
```

Proceed by typing the numbers in the string following each with [Enter]. The end of a string is indicated by [Enter] with no character.

```
ENTER ANALYSIS NUMBERS
#? 1
#? 2
#? 5
#? 8
#? 22
#? 15
#? 6
#?
```

This allows the maximum flexibility in selecting and ordering the analyses to be included in the data set, however it is frequently the case that the data in the buffer is already organized in rational sequences. If you include a negative number in the input sequence, then the program includes all numbers back to the previous entry. The following example specifies the set - 1,2,3,4,5,6,7,8,9,10,18,15,16 .

```
ENTER ANALYSIS NUMBERS
#? 1
#? -10
#? 18
#? 15
#? 16
#?
```

A special character (&) can be used to end the input of one number set and begin another. If you are producing a number of tables using the same formula and if they are long tables, it may be advantageous to enter all of them in a queue before starting the processing and printing. The following example produces two tables with five analyses each -

```
ENTER ANALYSIS NUMBERS
#? 1
#? 2
#? 3
#? 4
#? 5
#? &
#? 1
#? -5
#?
```

Each analyses has an eight character label associated with it. A special character (*) can be included in the number set to call for analyses based on the contents of the labels. The following example produces a table that includes numbers one to five, all analyses with BI as the first two characters in the label and ends with analyses 22 -

```
ENTER ANALYSIS NUMBERS
#? 1
#? -5
#? *
ENTER WILDCARDED LABEL TO BE USED (8 char.): BI******
#? 22
#?
```

COMMAND DESCRIPTIONS

1) CHOOSE A FORMULA

Displays a list of pre-prepared (stored) formulae in the presently active formula directory. Prompts you to load a replacement for the current formula. Choose by entering the formula number. An outline of the selected formula is displayed as it is read into memory.

This command is also used to display a directory of the stored formulae in the presently active directory, without loading a replacement for the current formula. If you enter a blank, then you return to the menu without disturbing the current formula. For a hard copy of the directory see p) PRINT FORMULA DIRECTORY in the utility options sub-menu.

Provision has been made for multiple directories of stored formulae, each directory with a capacity of 100 definitions and each with a four character password. The password of the active formula directory is shown in brackets in the title line of its displayed directory.

The formula directory password is always set to GSC1 at run-time. The installation copy of the program has a set of frequently used formulae stored in the GSC1 directory. The formulae used in this documentation are stored with DOCU as a password.

See 99) CHANGE FORMULA DIRECTORY for more details on the use of multiple formula storage areas and their passwords.

```
*1

                STORED FORMULAE (DOCU)

 1 Feldspar       2 Feldspar #1     3 Feldspar #2     4 Feldspar #3
 5 Feldspar #4    6 Feldspar #5     7 Colusite #1     8 Colusite #2
 9 Chalcopyr #1  10 Chalcopyr #2   11 Scapolite #1   12 Scapolte #2
13 Sodalite #1   14 Sodalite #2    15 Analcime #1    16 Analcime #2
17 Phlogopite #1 18 Phlogopite #2  19 Phlogopite #3  20 Garnet #1
21 Serpentine #1 22 Serpentine #2  23 Serpentine #3  24 Chromite #1
25 Amphibole #1  26 Amphibole #2   27 Amphibole #3   28 Amphibole #4
29 Amphibole #5  30 Smectite #1    31 Smectite #2    32 Smectite #3
33 Tourmaline #1 34 Tourmaline #2

RECALL WHICH FORMULA?: 1


    SAMPLE    Feldspar          VALUES TO BE OUTPUT
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  32 OX            WT.%  MOL.%
SIO2     .00    .000   SI    .000              Ab    .00    .00
AL2O3    .00    .000   AL    .000              An    .00    .00
NA2O     .00    .000              16.000       Or    .00    .00
CAO      .00    .000   NA    .000                  ------
K2O      .00    .000   CA    .000           TOTAL    .00
FEO      .00    .000   K     .000                  ------
      ------  ------               4.000
TOTAL    .00    .000   FE    .000
      ------  ------               1.000

PRESS ENTER FOR THE MENU:
```

2) ENTER A NEW FORMULA

The term **Formula** is used to encompass all the details of how the analyses are to be recalculated and what the format of the table is to be. Within this context a formula can include -

1) The elements in the analysis.

2) The order that the elements appear in the table.

3) Oxide or element format.

4) Valence of the oxides.

5) Fe as FeO or Fe_2O_3 or both.

6) Stoichiometric Fe^{+2} or Fe^{+3}.

7) The number of sites and cation total for the iron calculation.

8) Basis of normalization for the formula. This may be on total cations, cations in some sites, total oxygens, total oxygen and oxygen equivalents of negatively charged species or total anionic species.

9) Boundaries of formula sites in the element list.

10) Elements to be shared between sites. The elements are shared by defining an order of site filling.

11) Definitions of end member molecules to be calculated as mol % and/or weight % values.

12) Definitions of mol.% cation ratios to be used as plotting co-ordinates.

The process of entering this information is accomplished in three distinct steps -

a) The basic formula is entered in the form of a character string that is the same as a mineral formula written with bracket site delimiters and subscripts. (1 to 10 above) The program allows for up to 20 analyzed elements to be involved in the formula. This is reduced to 19 if the oxide option is chosen.

b) Up to 20 end member definitions are entered in the form of chemical formulae. (11 above)

c) Up to 20 cation ratio definitions are entered in a format specified by internal program prompts. (12 above)

The 2) ENTER A NEW FORMULA command automatically chains to 7) SPECIFY END MEMBERS and 8) SPECIFY RATIOS. These commands are described later in the chapter. You have the option to bypass the entry of end members and ratios at this point and append them later. In cases where the entry of the basic formula is complex or lengthy, it is prudent to delay the entry of end member and ratio definitions until a copy of the basic formula has been saved (3) SAVE CURRENT FORMULA). You are then backed up if something nasty happens when you try to compose end members or ratios.

The following syntax illustrations include a portion where the formula details are specified (2) ENTER A NEW FORMULA), and often a portion where the result is verified (33) ENTER WT.%). After the basic formula has been entered, the program displays an example of the format using zero values. This portion of the display interaction is reproduced in the first two illustrations and is omitted in subsequent illustrations where real values have been entered to verify the format. The worked examples of formula calculation and the calculation of stoichiometric Fe+2/Fe+3 contained in Appendices B and C are the basis of many of the illustrations.

Syntax Notes

1) Elements are entered using upper and lower case ... H He Li Be etc.

2) The order of the elements in the input string determines the order in the output.

3) Formula sites are indicated with opening and closing brackets.

4) An element may not be mentioned twice in a site, except where Fe^{+2} and Fe^{+3} are being distinguished and except oxygen.

5) The element symbols may be separated by commas or spaces for convenience.

6) Subscript numbers must immediately follow an element symbol or a closing bracket. If a subscript is omitted, it is presumed to be one. Subscripts on elements within a bracketed site are ignored, except oxygen, in which case they are included in the summation of total oxygen.

7) Elements may be divided between adjacent sites by repeating the string of overlapped elements as the last elements in the preceding site and the first elements in the succeeding site.

8) If oxygen is mentioned in the element string, then you may choose oxide or non-oxide format. In oxide format, the analyzed elements are reported as oxides and oxygen is not an analyzed element. In non-oxide format, oxygen is an analyzed element and all elements are reported as wt.% metals.

9) If the analysis is being presented in non-oxide format, the formula is based (normalized) on a specified number of atoms. The common choices for this number are a) one atom, b) the total atoms in the formula or c) the total atoms in one or more of the formula sites.

10) If the analysis is being presented in oxide format, then you may choose to base (normalize) the formula on a specified number of atoms with the same options as in the non-oxide case. The more usual selection however is to base the calculation of these formulae on a specified number of oxygens. The program will default to the total of the entered oxygens.

11) The program treats OH^-, $CO3^{-2}$, and $SO4^{-2}$ as discrete entities.

12) When the halogens or any of OH^-, $CO3^{-2}$, and $SO4^{-2}$ are involved in the formula, and when oxygen has been chosen as the calculation basis, the program prompts for you to choose normalization to total (F,Cl,O,OH....) or alternatively normalization to total oxygen equivalents (Examples 3a, 3b, 4a and 4b, Appendix B). The first method is used when you have values available for water and/or hydroxide and the other anionic species. The second method is used when one or more of these values are not available, which is almost always the case in microprobe work.

13) Iron may be represented in the formula by the symbols Fe, Fe^{+2} and Fe^{+3}. If the formula is in non-oxide format, then only Fe may be used. If oxide format has been specified and you want to calculate iron values, then Fe^{+2} and Fe^{+3} must both be included and Fe may not be used. The occurrence of iron as one valence state only is stated by using Fe with the default valence set to the desired value (j) EDIT DEFAULT VALENCES).

Chalcopyr #1

```
*2

MINERAL NAME? :Chalcopyr #1
FORMULA? :CuFeS2
DIVIDE THE FORMULA INTO SITES? [Y]: N
HOW MANY ATOMS IN THE CALCULATED FORMULA?: 4
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


    SAMPLE    Chalcopyr #1     VALUES TO BE OUTPUT
--------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   4 AT
  CU     .00    .000
  FE     .00    .000
  S      .00    .000
      ------  ------
TOTAL    .00    .000
      ------  ------
SAVE THIS FORMULA? [N]: Y
FORMULA IS NAMED Chalcopyr #1
CHANGE? [N]:


*33


LABEL?: CuFeS2
ENTER WT.% ELEMENTS   (Include decimal)
   CU?:34.54
   FE?:30.66
   S ?:35.02
      CuFeS2
--------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   4 AT
  CU   34.54    .995
  FE   30.66   1.005
  S    35.02   2.000
      ------  ------
TOTAL 100.22   4.000
      ------  ------
HARD COPY? [N]:
SAVE? [N]: Y
#  1  SAVED AS : CuFeS2
FINISHED? [N]: Y
```

Orthoclase Feldspar #1

```
*2

MINERAL NAME? :Feldspar #1
FORMULA? :Si,Al,Na,Ca,K,Fe,O
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]: N
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


    SAMPLE    Feldspar #1     VALUES TO BE OUTPUT
--------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   1 OX
SIO2     .00    .000
AL2O3    .00    .000
NA2O     .00    .000
CAO      .00    .000
K2O      .00    .000
FEO      .00    .000
      ------  ------
TOTAL    .00    .000
      ------  ------

SAVE THIS FORMULA? [N]: Y
FORMULA IS NAMED Feldspar #1
CHANGE? [N]:


*6

ENTER NEW NORMALIZATION BASIS: 8


*3

FORMULA IS NAMED Feldspar #1
CHANGE? [N]:
Feldspar #1        : ALREADY SAVED
REPLACE? [Y/N]: Y
```

```
*33

ENTER AS % OXIDES? [N]: Y
LABEL?: Orthocl
ENTER WT.% OXIDES     (Include decimal)
SIO2 ?:64.84
AL2O3?:17.42
NA2O ?:.78
CAO  ?:
K2O  ?:15.25
FEO  ?:.98


      Orthocl
------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   8 OX
SIO2   64.84   3.020
AL2O3  17.42    .956
NA2O     .78    .070
CAO      .00    .000
K2O    15.25    .906
FEO      .98    .038
       ------  ------
TOTAL  99.27   4.990
       ------  ------

HARD COPY? [N]:
SAVE? [N]: Y
#  2  SAVED AS : Orthocl
FINISHED? [N]: Y
```

Orthoclase Feldspar #2

```
*2

MINERAL NAME? :Feldspar #2
FORMULA? :(Na,Ca,K)4(Al,Si)16O32
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


    SAMPLE    Feldspar #2      VALUES TO BE OUTPUT
------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  32 OX
NA2O     .00    .000   NA    .000
CAO      .00    .000   CA    .000
K2O      .00    .000   K     .000
AL2O3    .00    .000              4.000
SIO2     .00    .000   AL    .000
       ------  ------   SI    .000
TOTAL    .00    .000             16.000
       ------  ------

SAVE THIS FORMULA? [N]: Y
FORMULA IS NAMED Feldspar #2
CHANGE? [N]:
```

Orthoclase Feldspar #3

```
*2

MINERAL NAME? :Feldspar #3
FORMULA? :(Si,Al)16(Na,Ca,K)4(Fe)O32
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


*33

ENTER AS % OXIDES? [N]: Y
LABEL?: Orthocl
ENTER WT.% OXIDES     (Include decimal)
SIO2 ?:64.84
AL2O3?:17.42
NA2O ?:.78
CAO  ?:
K2O  ?:15.25
FEO  ?:.98


      Orthocl
-------------------------------------------------------------------------------
        WT.%   ATOMS      CALC ON  32 OX
SIO2   64.84  12.078   SI  12.078
AL2O3  17.42   3.825   AL   3.825
NA2O     .78    .282              15.903
CAO      .00    .000   NA    .282
K2O    15.25   3.624   CA    .000
FEO      .98    .153   K    3.624
      ------  ------              3.906
TOTAL  99.27  19.962   FE    .153
      ------  ------               .153

HARD COPY? [N]:
SAVE? [N]:
FINISHED? [N]: Y
```

Colusite #1

A non-oxide mineral calculated on the basis of the total atoms in the formula and divided into sites.

```
*2

MINERAL NAME? :Colusite #1
FORMULA? :(Cu,Fe,Zn)13V(Sn,As)3(Se,S)16
DIVIDE THE FORMULA INTO SITES? [Y]:
SCALE FORMULA TO THE ATOMS IN ALL SITES? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N
```

Colusit

	WT.%	ATOMS	CALC ON	33 AT
CU	47.80	13.016	CU 13.016	
FE	.30	.093	FE .093	
ZN	.70	.185	ZN .185	
V	3.30	1.121		13.294
SN	9.00	1.312	V 1.121	
AS	7.30	1.686		1.121
SE	2.40	.526	SN 1.312	
S	27.90	15.060	AS 1.686	
				2.998
TOTAL	98.70	32.999	SE .526	
			S 15.060	
				15.586

Colusite #2

There are occasions where it is useful to base the formula on the atoms in one or more, but not all the formula sites. This can happen with defect structures, when the determined values for some elements are not as reliable as the others or when the crystal chemistry is poorly understood.

```
*2

MINERAL NAME? :Colusite #2
FORMULA? :(Cu,Fe,Zn)13V(Sn,As)3(Se,S)16
DIVIDE THE FORMULA INTO SITES? [Y]:
SCALE FORMULA TO THE ATOMS IN ALL SITES? [Y]: N
USE SITE  1 TO NORMALIZE THE FORMULA? [Y]: N
USE SITE  2 TO NORMALIZE THE FORMULA? [Y]: N
USE SITE  3 TO NORMALIZE THE FORMULA? [Y]: N
USE SITE  4 TO NORMALIZE THE FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


     Colusit
-------------------------------------------------------------------------------
       WT.%   ATOMS     CALC ON  16 AT*
  CU   47.80  13.362   CU  13.362
  FE     .30    .095   FE    .095
  ZN     .70    .190   ZN    .190
  V     3.30   1.151              13.647
  SN    9.00   1.347   V    1.151
  AS    7.30   1.731              1.151
  SE    2.40    .540   SN   1.347
  S    27.90  15.460   AS   1.731
     ------  ------              3.078
TOTAL  98.70  33.876   SE    .540
     ------  ------   S   15.460
                                16.000
    * SCALED TO  16 ATOM(S) IN SITE(S)   4
```

Sodalite #1

Calculated on the equivalent of 25 oxygens and then calculated on the basis of 26(O,Cl) in the next example. These are identical because no oxygen bearing radicals (OH^-, $CO3^{-2}$, $SO4^{-2}$, ...) are involved.

```
*2

MINERAL NAME? :Sodalite #1
FORMULA? :Na8Al6Si6O24Cl2
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]: N
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,CL)? [N]:
WHAT IS THE TOTAL (CL) IN THE FORMULA?: 2
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


      Sodalit
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  25 OX
NA2O   25.58   7.998
AL2O3  31.56   5.998
SIO2   37.22   6.002
  CL    7.32   2.001
      ------  ------
TOTAL 101.68  21.999
      ------  ------
TOT-O 100.03
```

Sodalite #2

Calculated on the equivalent of 25 oxygens in the previous example and here calculated on the basis of 26(O,Cl). These are identical because no oxygen bearing radicals (OH^-, $CO3^{-2}$, $SO4^{-2}$, ...) are involved.

```
*2

MINERAL NAME? :Sodalite #2
FORMULA? :Na8Al6Si6O24Cl2
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]: N
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,CL)? [N]: Y
WHAT IS THE TOTAL (O,CL) IN THE FORMULA?: 26
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


      Sodalit
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  26 OX*
NA2O   25.58   7.998
AL2O3  31.56   5.998
SIO2   37.22   6.002
  CL    7.32   2.001
      ------  ------
TOTAL 101.68  21.999
      ------  ------
TOT-O 100.03

* SCALED TO  26 (O,CL)
```

Serpentine #1

This example illustrates the inclusion of a water determination in the calculations. The values for Fe^{+2} and Fe^{+3} are also analytically determined, that is they are not estimated using stoichiometry. Since water and the iron oxidation state cannot be determined on a microprobe, they must be analyzed by some other method.

```
*2

MINERAL NAME? :Serpentine #1
FORMULA? :(Si,Al,Fe+3)2(Fe+2,Mg,K)3O5(OH)4
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,OH)? [N]: Y
WHAT IS THE TOTAL (O,OH) IN THE FORMULA?: 9
DO YOU WANT FE PARTITIONED BY STOICHIOMETRY? [N]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


      Serp#1
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   9 OX*
SIO2   41.97   1.939   SI   1.939
AL2O3    .10    .005   AL    .005
FE2O3    .38    .013   FE+3  .013
FEO     1.57    .061               1.957
MGO    42.50   2.926   FE+2  .061
K2O      .08    .005   MG   2.926
H2O    13.65   4.211   K     .005
       ------  ------              2.992
TOTAL 100.25   9.160   OH   4.211
       ------  ------              4.211

* SCALED TO   9 (O,OH)
```

Serpentine #2

The following is the same Serpentine that was given in the previous example, but now the analysis does not include water and Fe is expressed as FeO. The formula is now based on the hypothetical number of oxygens required for charge balance.

```
*2

MINERAL NAME? :Serpentine #2
FORMULA? :(Si,Al)2(Fe,Mg,K)3O7
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


      Serp#2
--------------------------------------------------------------------------------
       WT.%   ATOMS     CALC ON   7 OX
SIO2   41.97   1.970   SI   1.970
AL2O3    .10    .006   AL    .006
FEO     1.91    .075              1.976
MGO    42.50   2.974   FE    .075
K2O      .08    .005   MG   2.974
      ------  ------   K     .005
TOTAL  86.56   5.030              3.054
      ------  ------
```

Serpentine #3

The following formula is based on the hypothetical number of oxygens required for charge balance and uses analyzed values for iron in its two oxidation states. It is included to illustrate that calculations based on total anionic species (Serpentine #1) and calculations based on the number of oxygens for charge balance do not give precisely the same result when $(OH)^-$ is involved.

```
*2

MINERAL NAME? :Serpentine #3
FORMULA? :(Si,Al,Fe+3)2(Fe+2,Mg,K)3O5(OH)4
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,OH)? [N]:
WHAT IS THE TOTAL (OH) IN THE FORMULA?: 4
DO YOU WANT FE PARTITIONED BY STOICHIOMETRY? [N]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


      Serp#1
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   7 OX
SIO2   41.97   1.968   SI   1.968
AL2O3    .10    .006   AL    .006
FE2O3    .38    .013   FE+3  .013
FEO     1.57    .062                1.987
MGO    42.50   2.971   FE+2  .062
K2O      .08    .005   MG   2.971
H2O    13.65   4.275   K     .005
       ------  ------               3.038
TOTAL 100.25   9.300   OH   4.275
       ------  ------               4.275
```

Analcime #1

Calculation involving zeolitic water where a water determination is available.

```
*2

MINERAL NAME? :Analcime #1
FORMULA? :NaAlSi2O6.H2O
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]: N
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N

      Ancm#1
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   7 OX
NA2O   13.02    .912
AL2O3  22.21    .946
SIO2   56.42   2.039
H2O     8.67   2.092
      ------  ------
TOTAL 100.32   5.989
      ------  ------
```

Analcime #2

Calculation on an anhydrous basis of a mineral that has zeolitic water.

```
*2

MINERAL NAME? :Analcime #2
FORMULA? :NaAlSi2O6
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]: N
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N

      Ancm#2
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   6 OX
NA2O   13.02    .920
AL2O3  22.21    .954
SIO2   56.42   2.055
      ------  ------
TOTAL  91.65   3.929
      ------  ------
```

Phlogopite #1

This example includes a variety of features including the division of elements into formula sites, the sharing of an element between sites and the effect of anionic substitutions. Here it is scaled to the total number of anions.

```
*2

MINERAL NAME? :Phlogopite #1
FORMULA? :(Si,Al,Ti)8(Ti,Fe,Mn,Mg)6(Na,K)2O2O(OH,F)4
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,F ,OH)? [N]: Y
WHAT IS THE TOTAL (O,F ,OH) IN THE FORMULA?: 24
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N
```

	Phlog#1				
	WT.%	ATOMS		CALC ON	24 OX*
SIO2	41.18	5.825	SI	5.825	
AL2O3	12.52	2.088	AL	2.088	
TIO2	.99	.105	TI	.087	
FEO	.30	.035			8.000
MNO	.04	.005	TI	.018	
MGO	27.32	5.761	FE	.035	
NA2O	.88	.241	MN	.005	
K2O	11.93	2.153	MG	5.761	
H2O	1.06	1.001			5.819
F	6.74	3.015	NA	.241	
	---	---	K	2.153	
TOTAL	102.96	20.229			2.394
	---	---	OH	1.001	
TOT-O	100.12		F	3.015	
					4.016

* SCALED TO 24 (O,F ,OH)

Phlogopite #2

The same as above, but now scaled to 22 oxygen equivalents.

```
*2

MINERAL NAME? :Phlogopite #2
FORMULA? :(Si,Al,Ti)8(Ti,Fe,Mn,Mg)6(Na,K)2O22
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N
```

Phlog#2

	WT.%	ATOMS		CALC ON	22 OX
SIO2	41.18	5.828	SI	5.828	
AL2O3	12.52	2.088	AL	2.088	
TIO2	.99	.105	TI	.084	
FEO	.30	.036			8.000
MNO	.04	.005	TI	.021	
MGO	27.32	5.763	FE	.036	
NA2O	.88	.241	MN	.005	
K2O	11.93	2.154	MG	5.763	
					5.825
TOTAL	95.16	16.220	NA	.241	
			K	2.154	
					2.395

Phlogopite #3

Fluorine may be analyzed on a microprobe, but not water. The fluorine may be carried in the calculation and may still scale the formula on the basis of oxygen equivalents.

```
*2

MINERAL NAME? :Phlogopite #3
FORMULA? :(Si,Al,Ti)8(Ti,Fe,Mn,Mg)6(Na,K)2O2OF4
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,F )? [N]:
WHAT IS THE TOTAL (F ) IN THE FORMULA?: 4
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N

      Phlog#3
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  22 OX
SIO2   41.18   5.828   SI   5.828
AL2O3  12.52   2.088   AL   2.088
TIO2     .99    .105   TI    .084
FEO      .30    .036              8.000
MNO      .04    .005   TI    .021
MGO    27.32   5.763   FE    .036
NA2O     .88    .241   MN    .005
K2O    11.93   2.154   MG   5.763
  F     6.74   3.017              5.825
      ------  ------   NA    .241
TOTAL 101.90  19.237   K    2.154
      ------  ------              2.395
TOT-O  99.06           F    3.017
                                  3.017
```

Scapolite #1

This example introduces the treatment of CO_3^- and SO_4^- radicals.

```
*2

MINERAL NAME? :Scapolite #1
FORMULA? :(Si,Al)12(Ti,Fe+3,Mg,Fe+2,Mn,Na,Ca,K)4O24(OH,CO3,SO4,F,Cl)
CALCULATE AS OXIDES? [Y]:
(Si,Al)12(Ti,Fe+3,Mg,Fe+2,Mn,Na,Ca,K)4O24(OH,CO3 ????
IS THIS A CO3 RADICAL? [N]: Y
(Si,Al)12(Ti,Fe+3,Mg,Fe+2,Mn,Na,Ca,K)4O24(OH,CO3,SO4 ????
IS THIS AN SO4 RADICAL? [N]: Y
DIVIDE THE FORMULA INTO SITES? [Y]: Y
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,F ,CL,OH,CO3,SO4)? [N]:
WHAT IS THE TOTAL (F ,CL,OH,CO3,SO4) IN THE FORMULA?: 1
DO YOU WANT FE PARTITIONED BY STOICHIOMETRY? [N]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N
```

Scapol

	WT.%	ATOMS	CALC ON	49 OX	
SIO2	52.10	15.383	SI	15.383	
AL2O3	23.79	8.280	AL	8.280	
TIO2	.02	.004			23.663
FE2O3	.23	.051	TI	.004	
MGO	.18	.079	FE+3	.051	
FEO	.00	.000	MG	.079	
MNO	.00	.000	FE+2	.000	
NA2O	6.86	3.928	MN	.000	
CAO	11.13	3.521	NA	3.928	
K2O	.87	.328	CA	3.521	
H2O	.07	.138	K	.328	
CO2	2.14	.863			7.911
SO3	.80	.177	OH	.138	
F	.11	.103	CO3	.863	
CL	1.85	.926	SO4	.177	
	------	------	F	.103	
TOTAL	100.15	33.781	CL	.926	
	------	------			2.207
TOT-O	99.69				

Scapolite #2

An analysis in oxide format with a formula based a specified number of atoms in the first site.

```
*2

MINERAL NAME? :Scapolite #2
FORMULA? :(Si,Al)12(Ti,Fe+3,Mg,Fe+2,Mn,Na,Ca,K)4O24(OH,CO3,SO4,F,Cl)
CALCULATE AS OXIDES? [Y]:
(Si,Al)12(Ti,Fe+3,Mg,Fe+2,Mn,Na,Ca,K)4O24(OH,CO3 ????
IS THIS A CO3 RADICAL? [N]: Y
(Si,Al)12(Ti,Fe+3,Mg,Fe+2,Mn,Na,Ca,K)4O24(OH,CO3,SO4 ????
IS THIS AN SO4 RADICAL? [N]: Y
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]: N
SCALE FORMULA TO THE ATOMS IN ALL SITES? [Y]: N
USE SITE  1 TO NORMALIZE THE FORMULA? [Y]:
USE SITE  2 TO NORMALIZE THE FORMULA? [Y]: N
USE SITE  3 TO NORMALIZE THE FORMULA? [Y]: N
USE SITE  4 TO NORMALIZE THE FORMULA? [Y]: N
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N

      Scapol
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  12 AT*
SIO2   52.10   7.801   SI   7.801
AL2O3  23.79   4.199   AL   4.199
TIO2     .02    .002             12.000
FE2O3    .23    .026   TI    .002
MGO      .18    .040   FE+3  .026
FEO      .00    .000   MG    .040
MNO      .00    .000   FE+2  .000
NA2O    6.86   1.992   MN    .000
CAO    11.13   1.786   NA   1.992
K2O      .87    .166   CA   1.786
H2O      .07    .070   K     .166
CO2     2.14    .438              4.012
SO3      .80    .090   OH    .070
  F      .11    .052   CO3   .438
  CL    1.85    .470   SO4   .090
      ------  ------   F     .052
TOTAL 100.15  17.132   CL    .470
      ------  ------              1.120
TOT-O  99.69

    * SCALED TO  12 ATOM(S) IN SITE(S)   1
```

Tourmaline #1

Calculated to include determinations of the light elements.

```
*2

MINERAL NAME? :Tourmaline #1
FORMULA? :(Si,B,Al)15(Al,Mg,Ti,Fe,Na,Ca,K)4027(OH)4
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT THE FORMULA BASED ON TOTAL (O,OH)? [N]: Y
WHAT IS THE TOTAL (O,OH) IN THE FORMULA?: 31
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N
```

	Tourm#1				
	WT.%	ATOMS		CALC ON	31 OX*
SIO2	35.96	5.759	SI	5.759	
B2O3	10.73	2.966	B	2.966	
AL2O3	30.85	5.823	AL	5.823	
MGO	13.67	3.263			14.548
TIO2	.14	.017	AL	.000	
FEO	.76	.102	MG	3.263	
NA2O	1.63	.506	TI	.017	
CAO	2.41	.414	FE	.102	
K2O	.09	.018	NA	.506	
H2O	4.16	4.448	CA	.414	
	---	---	K	.018	
TOTAL	100.40	23.316			4.320
	---	---	OH	4.448	
					4.448

* SCALED TO 31 (O,OH)

Tourmaline #2

Calculated without the light elements.

```
*2

MINERAL NAME? :Tourmaline #2
FORMULA? :(Si,Al)24(Al,Mg,Ti,Fe,Na,Ca,K)8049
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N

      Tourm#2
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  49 OX
SIO2   35.96  11.599   SI  11.599
AL2O3  30.85  11.729   AL  11.729
MGO    13.67   6.573              23.328
TIO2     .14    .034   AL    .000
FEO      .76    .205   MG   6.573
NA2O    1.63   1.019   TI    .034
CAO     2.41    .833   FE    .205
K2O      .09    .037   NA   1.019
      ------  ------   CA    .833
TOTAL  85.51  32.029   K     .037
      ------  ------              8.701
```

Amphibole #1

This demonstrates the division of total Fe into Fe^{+2} and Fe^{+3} by assuming an ideal number of cations in formula sites (Appendix C). Here total Fe is entered as FeO.

```
*2

MINERAL NAME? :Amphibole #1
FORMULA? :(Si,Ti,Al)8(Al,Fe+3,Fe+2,Mn,Mg)5(Ca,Na,K)2023
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT FE PARTITIONED BY STOICHIOMETRY? [N]: Y
FORCE STOICHIOMETRY IN SITE  1? [N]:Y
FORCE STOICHIOMETRY IN SITE  2? [N]:Y
FORCE STOICHIOMETRY IN SITE  3? [N]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


*33

LABEL?: Amph#1
ENTER WT.% OXIDES     (Include decimal)
SIO2 ?:52.78
TIO2 ?:.43
AL203?:5.77
FE203?:0.00
FEO  ?:8.81
MNO  ?:.17
MGO  ?:17.43
CAO  ?:11.9
NA2O ?:.68
K2O  ?:.07
```

Amph#1

	WT.%	ATOMS	CALC ON	23 OX
SIO2	52.78	7.347	SI 7.347	
TIO2	.43	.045	TI .045	
AL2O3	5.77	.947	AL .608	
FE2O3	4.98	.521		8.000
FEO	4.33	.504	AL .339	
MNO	.17	.020	FE+3 .521	
MGO	17.43	3.616	FE+2 .504	
CAO	11.90	1.775	MN .020	
NA2O	.68	.184	MG 3.616	
K2O	.07	.012		5.000
TOTAL	98.54	14.971	CA 1.775	
			NA .184	
			K .012	
				1.971

3) SAVE CURRENT FORMULA

Copies the current formula to the formula directory. This is how you archive a newly created formula for future use. The formula is given a 16 character name. You may overwrite an older formula in storage by providing a duplicate name.

See also 99) CHANGE FORMULA DIRECTORY.

```
*3

FORMULA IS NAMED Feldspar
CHANGE?: y
NEW NAME?: Newfeld

or

FORMULA IS NAMED Feldspar
CHANGE?: n
Feldspar          : ALREADY SAVED
REPLACE? Y/N: y

etc
```

4) DELETE FORMULA

Deletes a formula in the formula directory. This does not disturb the current formula. Choose the formula to be deleted by number.

See also 99) CHANGE FORMULA DIRECTORY.

```
*4

                STORED FORMULAE (DOCU)

  1 Feldspar        2 Feldspar #1     3 Feldspar #2     4 Feldspar #3
  5 Feldspar #4     6 Feldspar #5     7 Colusite #1     8 Colusite #2
  9 Chalcopyr #1   10 Chalcopyr #2   11 Scapolite #1   12 Scapolte #2
 13 Sodalite #1    14 Sodalite #2    15 Analcime #1    16 Analcime #2
 17 Phlogopite #1  18 Phlogopite #2  19 Phlogopite #3  20 Garnet #1
 21 Serpentine #1  22 Serpentine #2  23 Serpentine #3  24 Chromite #1
 25 Amphibole #1   26 Amphibole #2   27 Amphibole #3   28 Amphibole #4
 29 Amphibole #5   30 Smectite #1    31 Smectite #2    32 Smectite #3
 33 Tourmaline #1  34 Tourmaline #2  35 Newfeld
DELETE WHICH FORMULA?: 35

*1

                STORED FORMULAE (DOCU)

  1 Feldspar        2 Feldspar #1     3 Feldspar #2     4 Feldspar #3
  5 Feldspar #4     6 Feldspar #5     7 Colusite #1     8 Colusite #2
  9 Chalcopyr #1   10 Chalcopyr #2   11 Scapolite #1   12 Scapolte #2
 13 Sodalite #1    14 Sodalite #2    15 Analcime #1    16 Analcime #2
 17 Phlogopite #1  18 Phlogopite #2  19 Phlogopite #3  20 Garnet #1
 21 Serpentine #1  22 Serpentine #2  23 Serpentine #3  24 Chromite #1
 25 Amphibole #1   26 Amphibole #2   27 Amphibole #3   28 Amphibole #4
 29 Amphibole #5   30 Smectite #1    31 Smectite #2    32 Smectite #3
 33 Tourmaline #1  34 Tourmaline #2

RECALL WHICH FORMULA?:
```

5) DISPLAY CURRENT FORMULA

Displays an outline of the current formula, organized so that all the output items will fit on the monitor. These same items are arranged in columns when a table is produced. The following is an amphibole format that we use frequently.

This display is intended to present the details of the output format and not the internal factors that determine how iron oxidation ratios, cation ratios and end-member components are calculated. These parameters may be printed with k) DISPLAY FORMULA CODES.

```
*5

   SAMPLE    Amphibole #5     VALUES TO BE OUTPUT
-------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  23 OX                          RATIO
SIO2     .00    .000   SI    .000                          Fm  .000
AL2O3    .00    .000   AL    .000
TIO2     .00    .000               8.000
CR2O3    .00    .000   AL    .000
FE2O3    .00    .000   TI    .000
FEO      .00    .000   CR    .000
MNO      .00    .000   FE+3  .000
MGO      .00    .000   FE+2  .000
CAO      .00    .000   MN    .000
NA2O     .00    .000   MG    .000
K2O      .00    .000               5.000
  F      .00    .000   CA    .000
  CL     .00    .000   NA    .000
       ------  ------             2.000
TOTAL    .00    .000   NA    .000
       ------  ------   K     .000
TOT-O    .00                      1.000
                        F     .000
                        CL    .000
                                 2.000
PRESS ENTER FOR THE MENU:
```

6) CHANGE FORMULA BASIS

A normalization number is needed in all formula calculations (Appendix B) and this menu item may be used to change it.

Warning: Using this option may have unpredictable consequences in more complex formulae. In these cases it is advisable to change the normalization by re-declaring the entire formula and any end members (3) ENTER A NEW FORMULA, 7) SPECIFY END MEMBERS). These problems can occur when the calculations involve normalization to less than the total in all sites, Fe^{+2} and Fe^{+3} calculations or end member calculations.

7) SPECIFY END MEMBERS

This option provides the opportunity to define up to 20 molecular end-members that will be part of the output. These are useful as plotting co-ordinates on various standard mineralogical diagrams. A table of wt.% of end-members can be a highly sensitive test of the quality of an analysis.

Each end-member label is a five character field. Entering a blank label terminates the option.

End-members are entered as a chemical formula using the syntax rules given in 2) ENTER A NEW FORMULA with some restrictions. The first restriction is that the end-member formulae must be on the same basis as the original defining formula. For example, if a feldspar format is defined as (Na,Ca,K)4(Si,Al)12O32 then Na4Al4Si12O32 is a valid end-member and NaAlSi3O8 is not. The second restriction is that the end-member may not have unspecified substitutions in any site. In the feldspar example this means that Na4Al4Si12O32 is a valid end-member and Na4(Al,Si)16O32 is not.

During the definition process you are asked to specify the principal element in each end-member. The calculation proceeds by first assuming that the content of the principal element represents the end-member and then subtracting the amount of this element involved in other end-members (Appendix B). In the simplest situations, each end-member may be represented by an element that is unique to the end-member (e.g. Feldspar). In other cases you are forced by the complexity of the potential substitutions to assign a common principle element to a group of end-members (e.g. Chromite). This group of end-members must then be subdivided in an arbitrary proportion.

The program will attempt to automatically set up the correct factors to produce the desired result. No further operator intervention is required when the entered end-members are a mathematically complete summation of the potential variation in the mineral being described. There is an unpredictable level of complexity where the logic built into the program breaks down and you must opt for either a simpler treatment or manually provide the correct factors and calculation sequence with k) DISPLAY FORMULA CODES and 1) EDIT END MEMBER CODES.

It is a good practice to cross-check what the program is doing with some hand calculations. This will intercept errors and will help identify cases where the calculation that you expected exceeds the logic built into the program. End member calculations may also be verified by processing a trial composition that is equal parts of the theoretical end member molecules.

In some cases, it is necessary to define prerequisite ratios before defining end-members. This is accomplished with 8) SPECIFY RATIOS. An example of this is the case where the same principal element has been assigned to more than one end-member.

The order of calculation may become important in the more complex sets of end-member molecules. This happens when the defined end-members are not a complete description of the potential variation in the mineral. End-member sets of this type can still be used if caution is exercised and they are applied only to compositions inside their defined range.

Each end-member value is a function of the weight of its principal element modified by the weight of all other end-members that contain this element. Any end-member that depends in this way on other contributing end-member values has an associated error that increases with the number of contributing end-members. The greatest error will most likely be associated with the end-members that are latest in the calculation train. The Grossularite value in the Garnet example below has the greatest error load of all the defined end-members.

The examples given here follow the worked examples in Appendix B. Some minor differences appear in the results because of compounded rounding errors, especially where Fe values are being calculated.

Feldspar #4

```
*5

    SAMPLE    Feldspar #3      VALUES TO BE OUTPUT
-------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  32 OX
SIO2     .00    .000   SI    .000
AL2O3    .00    .000   AL    .000
NA2O     .00    .000              16.000
CAO      .00    .000   NA    .000
K2O      .00    .000   CA    .000
FEO      .00    .000   K     .000
      ------  ------               4.000
TOTAL    .00    .000   FE    .000
      ------  ------               1.000

PRESS ENTER FOR THE MENU:
```

```
*7

REPORT WT% END MEMBERS? [N]: Y


SITE #  1 HAS:
SI AL  SUBSCRIPT =  16
SITE #  2 HAS:
NA CA K   SUBSCRIPT =   4
SITE #  3 HAS:
FE  SUBSCRIPT =   1

LABEL FOR END MEMB.  1    :    Ab
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Na4Al4Si12O32
SI 12 AL  4 NA  4 O 32
WHICH IS THE KEY ELEMENT? : Na


SITE #  1 HAS:
SI AL  SUBSCRIPT =  16
SITE #  2 HAS:
NA CA K   SUBSCRIPT =   4
SITE #  3 HAS:
FE  SUBSCRIPT =   1

LABEL FOR END MEMB.  2    :    An
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Ca4Al8Si8O32
SI  8 AL  8 CA  4 O 32
WHICH IS THE KEY ELEMENT? : Ca


SITE #  1 HAS:
SI AL  SUBSCRIPT =  16
SITE #  2 HAS:
NA CA K   SUBSCRIPT =   4
SITE #  3 HAS:
FE  SUBSCRIPT =   1

LABEL FOR END MEMB.  3    :    Or
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
K4Al4Si12O32
SI 12 AL  4 K   4 O 32
WHICH IS THE KEY ELEMENT? : K


SITE #  1 HAS:
SI AL  SUBSCRIPT =  16
SITE #  2 HAS:
NA CA K   SUBSCRIPT =   4
SITE #  3 HAS:
FE  SUBSCRIPT =   1

LABEL FOR END MEMB.  4    :
```

```
      Labrad
-------------------------------------------------------------------------------
        WT.%   ATOMS      CALC ON  32 OX            WT.%  MOL.%
SIO2    51.90   9.449   SI   9.449          Ab   32.67  34.52
AL2O3   30.45   6.535   AL   6.535          An   64.70  64.42
NA2O     3.86   1.363             15.984     Or    1.07   1.06
CAO     13.04   2.544   NA   1.363            ------
K2O       .18    .042   CA   2.544     TOTAL  98.43
FEO       .35    .053   K     .042           ------
       ------  ------              3.949
TOTAL   99.78  19.986   FE    .053
       ------  ------                .053
```

Garnet #1

```
*2

MINERAL NAME? :Garnet #1
FORMULA? :(Si,Al,Fe+3)6(Al,Fe+3,Ti,Cr)4(Mg,Fe+2,Mn,Ca,K)6O24
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT FE PARTITIONED BY STOICHIOMETRY? [N]: Y
FORCE STOICHIOMETRY IN SITE  1? [N]:Y
FORCE STOICHIOMETRY IN SITE  2? [N]:Y
FORCE STOICHIOMETRY IN SITE  3? [N]:Y
SPECIFY RATIOS?      [Y\N]: Y

LABEL FOR RATIO  1:   Fmg


SITE #  1 HAS:
(a) SI (b) AL (c) FE+3
SITE #  2 HAS:
(e) AL (f) FE+3 (g) TI (h) CR
SITE #  3 HAS:
(j) MG (k) FE+2 (l) MN (m) CA (n) K

ENTER RATIO  1:     eg. ( 2a + c ) / ( 2a + b + c )
(c+f+k)/(c+f+j+k)

LABEL FOR RATIO  2:
SPECIFY END MEMBERS? [Y\N]: Y
REPORT WT% END MEMBERS? [N]: Y
```

```
SITE #  1 HAS:
(a) SI (b) AL (c) FE+3
SITE #  2 HAS:
(e) AL (f) FE+3 (g) TI (h) CR
SITE #  3 HAS:
(j) MG (k) FE+2 (l) MN (m) CA (n) K

LABEL FOR END MEMB.  1    : Alman
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
(Fe+2)6Al4Si6O24
SI  6 AL  4 FE+2  6 O 24
WHICH IS THE KEY ELEMENT? : Fe+2

LABEL FOR END MEMB.  2    : Andra
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Ca6(Fe+3)4Si6O24
SI  6 FE+3  4 CA  6 O 24
WHICH IS THE KEY ELEMENT? : Fe+3

LABEL FOR END MEMB.  3    : Schlm
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Ca6Ti4Si6O24
SI  6 TI  4 CA  6 O 24
WHICH IS THE KEY ELEMENT? : Ti

LABEL FOR END MEMB.  4    : Gross
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Ca6Al4Si6O24
SI  6 AL  4 CA  6 O 24
WHICH IS THE KEY ELEMENT? : Ca

LABEL FOR END MEMB.  5    : Pyrop
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Mg6Al4Si6O24
SI  6 AL  4 MG  6 O 24
WHICH IS THE KEY ELEMENT? : Mg

LABEL FOR END MEMB.  6    : Spess
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Mn6Al4Si6O24
SI  6 AL  4 MN  6 O 24
WHICH IS THE KEY ELEMENT? : Mn

LABEL FOR END MEMB.  7    : Uvaro
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Ca6Cr4Si6O24
SI  6 CR  4 CA  6 O 24
WHICH IS THE KEY ELEMENT? : Cr

LABEL FOR END MEMB.  8    :
```

```
*33

ENTER AS % OXIDES? [Y]:
LABEL?: Garn#1
ENTER WT.% OXIDES     (Include decimal)
SIO2 ?:37.76
AL2O3?:20.75
FE2O3?:
TIO2 ?:.14
CR2O3?:.07
MGO  ?:2.89
FEO  ?:30.301
MNO  ?:1.22
CAO  ?:7.52
K2O  ?:.04

      Garn#1
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  24 OX            WT.%  MOL.%          RATIO
SIO2   37.76   5.972   SI    5.972          Alman  67.31  64.54     Fmg  .855
AL2O3  20.75   3.868   AL     .028          Andra   4.09   3.84
FE2O3   1.28    .153   FE+3   .000          Schlm    .44    .43
TIO2     .14    .017                 6.000  Gross  15.89  16.83
CR2O3    .07    .009   AL    3.840          Pyrop   9.63  11.40
MGO     2.89    .681   FE+3   .153          Spess   2.83   2.73
FEO    29.15   3.855   TI     .017          Uvaro    .24    .23
MNO     1.22    .163   CR     .009                ------
CAO     7.52   1.274                 4.019  TOTAL 100.42
K2O      .04    .008   MG     .681                ------
      ------  ------   FE+2  3.855
TOTAL 100.82  16.000   MN     .163
      ------  ------   CA    1.274
                       K      .008
                                   5.981

HARD COPY? [N]:
SAVE? [N]:
FINISHED? [N]: Y
```

Chromite #1

```
*2

MINERAL NAME? :Chromite #1
FORMULA? :(Ti,Al,Cr,Fe+3)16(Fe+2,Mg,Mn)8O32
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]:
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
DO YOU WANT FE PARTITIONED BY STOICHIOMETRY? [N]: Y
FORCE STOICHIOMETRY IN SITE  1? [N]:Y
FORCE STOICHIOMETRY IN SITE  2? [N]:Y
SPECIFY RATIOS?      [Y\N]: Y
```

```
LABEL FOR RATIO  1:   Fmg


SITE #  1 HAS:
(a) TI (b) AL (c) CR (d) FE+3
SITE #  2 HAS:
(f) FE+2 (g) MG (h) MN

ENTER RATIO  1:     eg. ( 2a + c ) / ( 2a + b + c )
(f)/(f+g)

LABEL FOR RATIO  2:   Mfe
ENTER RATIO  2:     eg. ( 2a + c ) / ( 2a + b + c )
(g)/(f+g)

LABEL FOR RATIO  3:    Mg
ENTER RATIO  3:     eg. ( 2a + c ) / ( 2a + b + c )
(g)/(f+g+h)

LABEL FOR RATIO  4:    Fe
ENTER RATIO  4:     eg. ( 2a + c ) / ( 2a + b + c )
(f)/(f+g+h)

LABEL FOR RATIO  5:    Mn
ENTER RATIO  5:     eg. ( 2a + c ) / ( 2a + b + c )
(h)/(f+g+h)

LABEL FOR RATIO  6:
SPECIFY END MEMBERS? [Y\N]: Y
REPORT WT% END MEMBERS? [N]: Y

LABEL FOR END MEMB.  1    : Mgchr
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Mg8Cr16O32
CR 16 MG  8 O 32
WHICH IS THE KEY ELEMENT? : Cr

LABEL FOR END MEMB.  2    : Chrom
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
(Fe+2)8Cr16O32
CR 16 FE+2  8 O 32
WHICH IS THE KEY ELEMENT? : Cr

LABEL FOR END MEMB.  3    : Spinl
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Mg8Al16O32
AL 16 MG  8 O 32
WHICH IS THE KEY ELEMENT? : Al

LABEL FOR END MEMB.  4    : Hercy
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
(Fe+2)8Al16O32
AL 16 FE+2  8 O 32
WHICH IS THE KEY ELEMENT? : Al
```

```
LABEL FOR END MEMB.  5    : Galax
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Mn8Al16O32
AL 16 MN  8 O 32
WHICH IS THE KEY ELEMENT? : Al

LABEL FOR END MEMB.  6    : Mgnsf
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Mg8(Fe+3)16O32
FE+3 16 MG  8 O 32
WHICH IS THE KEY ELEMENT? : Fe+3

LABEL FOR END MEMB.  7    : Magnt
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
(Fe+2)8(Fe+3)16O32
FE+3 16 FE+2  8 O 32
WHICH IS THE KEY ELEMENT? : Fe+3

LABEL FOR END MEMB.  8    : Jacob
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
Mn8(Fe+3)16O32
FE+3 16 MN  8 O 32
WHICH IS THE KEY ELEMENT? : Fe+3

LABEL FOR END MEMB.  9    : Ulvsp
ENTER END MEMBER FORMULA:      (Include subscript for each element)
                                   eg. Ca2(Fe+2)3Al3Si7O22(OH)2
(Fe+2)16Ti8O32
TI  8 FE+2 16 O 32
WHICH IS THE KEY ELEMENT? : Ti

LABEL FOR END MEMB. 10    :


AL IS THE KEY ELEMENT IN  3 END MEMBERS.
IT MUST BE APPORTIONED WITH THE APPROPRIATE RATIO.

WHAT ARE THE RATIOS NEEDED TO APPORTION AL IN Spinl?: 3

WHAT ARE THE RATIOS NEEDED TO APPORTION AL IN Hercy?: 4

WHAT ARE THE RATIOS NEEDED TO APPORTION AL IN Galax?: 5

CR IS THE KEY ELEMENT IN  2 END MEMBERS.
IT MUST BE APPORTIONED WITH THE APPROPRIATE RATIO.

WHAT ARE THE RATIOS NEEDED TO APPORTION CR IN Mgchr?: 2

WHAT ARE THE RATIOS NEEDED TO APPORTION CR IN Chrom?: 1

FE+3 IS THE KEY ELEMENT IN  3 END MEMBERS.
IT MUST BE APPORTIONED WITH THE APPROPRIATE RATIO.

WHAT ARE THE RATIOS NEEDED TO APPORTION FE+3 IN Mgnsf?: 3

WHAT ARE THE RATIOS NEEDED TO APPORTION FE+3 IN Magnt?: 4

WHAT ARE THE RATIOS NEEDED TO APPORTION FE+3 IN Jacob?: 5
```

*33

Chrm#1

	WT.%	ATOMS	CALC ON	32 OX		WT.%	MOL.%		RATIO
TIO2	.93	.186	TI .186		Mgchr	16.90	17.58	Fmg	.635
AL2O3	14.43	4.528	AL 4.528		Chrom	34.24	30.59	Mfe	.365
CR2O3	36.61	7.707	CR 7.707		Spinl	7.29	10.25	Mg	.362
FE2O3	16.94	3.394	FE+3 3.394		Hercy	15.51	17.84	Fe	.630
FEO	23.17	5.160		15.815	Galax	.18	.20	Mn	.007
MGO	7.47	2.965	FE+2 5.160		Mgnsf	7.69	7.68		
MNO	.26	.059	MG 2.965		Magnt	15.48	13.37		
			MN .059		Jacob	.18	.15		
TOTAL	99.81	23.999		8.184	Ulvsp	2.60	2.32		
					TOTAL	100.07			

HARD COPY? [N]:
SAVE? [N]: Y
18 SAVED AS : Chrm#1
FINISHED? [N]: Y

8) SPECIFY RATIOS

This option provides the opportunity to define up to 20 cation ratios that will be part of the output. These are useful as plotting co-ordinates on various standard mineralogical diagrams. Ratios are necessary to complete the calculation of some end-members in (7) SPECIFY END MEMBERS).

The example below involves a simple ferromagnesian ratio. There are more detailed examples in the description of how to define end-members.

Each ratio label is a five character field. Entering a blank label terminates the option.

k) DISPLAY FORMULA CODES and m) EDIT RATIO CODES may be used to view and alter the definition of any existing ratio calculation.

Remember, you must save/resave the current routine if you want to retain the newly defined or altered ratios.

```
*1

                  STORED FORMULAE (DOCU)

  1 Feldspar        2 Feldspar #1     3 Feldspar #2     4 Feldspar #3
  5 Feldspar #4     6 Feldspar #5     7 Colusite #1     8 Colusite #2
  9 Chalcopyr #1   10 Chalcopyr #2   11 Scapolite #1   12 Scapolte #2
 13 Sodalite #1    14 Sodalite #2    15 Analcime #1    16 Analcime #2
 17 Phlogopite #1  18 Phlogopite #2  19 Phlogopite #3  20 Garnet #1
 21 Serpentine #1  22 Serpentine #2  23 Serpentine #3  24 Chromite #1
 25 Amphibole #1   26 Amphibole #2   27 Amphibole #3   28 Amphibole #4
 29 Amphibole #5   30 Smectite #1    31 Smectite #2    32 Smectite #3
 33 Tourmaline #1  34 Tourmaline #2

RECALL WHICH FORMULA?: 25

   SAMPLE    Amphibole #1     VALUES TO BE OUTPUT
-------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  23 OX
SIO2     .00    .000   SI    .000
TIO2     .00    .000   TI    .000
AL2O3    .00    .000   AL    .000
FE2O3    .00    .000               8.000
FEO      .00    .000   AL    .000
MNO      .00    .000   FE+3  .000
MGO      .00    .000   FE+2  .000
CAO      .00    .000   MN    .000
NA2O     .00    .000   MG    .000
K2O      .00    .000               5.000
      ------  ------   CA    .000
TOTAL    .00    .000   NA    .000
      ------  ------   K     .000
                                  2.000
PRESS ENTER FOR THE MENU:
```

*8

LABEL FOR RATIO 1: Fmg

SITE # 1 HAS:
(a) SI (b) TI (c) AL
SITE # 2 HAS:
(e) AL (f) FE+3 (g) FE+2 (h) MN (i) MG
SITE # 3 HAS:
(k) CA (l) NA (m) K

ENTER RATIO 1: eg. (2a + c) / (2a + b + c)
(f+g+h)/(f+g+h+i)

LABEL FOR RATIO 2:

*3

FORMULA IS NAMED Amphibole #1
CHANGE?: Y
NEW NAME?: Amphibole #2

Amph#1

	WT.%	ATOMS	CALC ON	23 OX		RATIO
SIO2	52.78	7.347	SI 7.347		Fmg	.224
TIO2	.43	.045	TI .045			
AL2O3	5.77	.947	AL .608			
FE2O3	5.01	.525		8.000		
FEO	4.30	.501	AL .339			
MNO	.17	.020	FE+3 .525			
MGO	17.43	3.616	FE+2 .501			
CAO	11.90	1.775	MN .020			
NA2O	.68	.183	MG 3.616			
K2O	.07	.012		5.001		
			CA 1.775			
TOTAL	98.54	14.971	NA .183			
			K .012			
				1.970		

9) UTILITY OPTIONS

This choice brings up the following sub-menu. The items here are identified by letters and you make your choice by entering the appropriate letter in response to the prompt. You may choose from this menu without displaying it. Enter any of these letters in response to the main menu prompt and the effect will be the same as if you had displayed the utility menu first.

```
*9

                GENERAL UTILITY COMMANDS
                ************************

   a ) PAGE EJECT                  j ) EDIT DEFAULT VALENCES
   b ) LINE FEED                   k ) DISPLAY FORMULA CODES
   c ) RESET (TOP OF FORM)         l ) EDIT END MEMBER CODES
   d ) COMPRESSED PRINT            m ) EDIT RATIO CODES
   e ) NORMAL PRINT                n )
   f ) STANDARD PAGE               o )
   g ) LEGAL PAGE                  p ) PRINT FORMULA DIRECTORY
   h ) NEW PRINTER CONTROL CODES   q )
   i ) SIGNIFICANT FIGURES         r ) RETURN TO MAIN MENU

*
```

Command descriptions for these items are given in this chapter after the descriptions of the items in the main menu.

a) PAGE EJECT

Issues a page eject control code to the printer. See h) NEW PRINTER CONTROL CODES.

b) LINE FEED

Issues a given number of line feeds to the printer. Enter the desired number of line feeds in response to the prompt. Press [Enter] with no number to return to the menu. See h) NEW PRINTER CONTROL CODES.

```
*b

#?5
#?
```

c) RESET (TOP OF FORM)

Issues a reset control code to the printer. This has the effect of returning the printer to its power on defaults including a reset of the top of form on continous feed printers. See h) NEW PRINTER CONTROL CODES.

d) COMPRESSED PRINT

Issues the control code that sets the printer to compressed print mode. See h) NEW PRINTER CONTROL CODES.

e) NORMAL PRINT

Issues the control code that sets the printer to normal print mode. See h) NEW PRINTER CONTROL CODES.

f) STANDARD PAGE

Issues the control code to set a standard page size on the printer. This setting only has meaning on sheet feeding printers. See h) NEW PRINTER CONTROL CODES.

g) LEGAL PAGE

Issues the control code to set a legal page size on the printer. This setting only has meaning on sheet feeding printers. See h) NEW PRINTER CONTROL CODES.

h) NEW PRINTER CONTROL CODES

This option gives you access to the parameters and control codes that are needed to manage the printer that you are using. They are stored in a disk file (PRNCOD) and are loaded when the program is run. Any change made with this command is written to the PRNCOD file and is therefore part of the configuration loaded at runtime.

The disk file (PRNCOD) contains two printer configurations and a flag that tells the program which configuration is to be loaded at runtime. One configuration is for a Roland[DG] PR-1215 printer and should work well with any standard dot matrix printer. The second configuration is for an HP LASERJET IIP. The distribution copy of the program has the flag set so that the dot matrix configuration is loaded.

A printer configuration consists of a series of parameters and printer control codes.

The parameters are -

1) Printer device or file name. (eg. PRN PRN: LPT LPT:) This is accessed only at run-time when the program cannot find the print device.
2) Printer type.
   DM - Dot matrix, continous feed paper
   LP - Laser, sheet feeding
3) Page size.
   S - Standard (DM and LP)
   L - Legal (LP only)
4) Page length in lines. (for S on DM, for S and L on LP)

The control codes are -

1) Printer reset. This is the same as a power off/on, which returns the printer to its default settings. In the case of a continous feed printer, this includes a top of form. This control code is also issued by the program on initialization and on exit in those cases where LP (Laser Printer) has been chosen as the printer type.

2) Page eject. This code is issued automatically before every page in output tables (22) OUTPUT RESULTS). It is also issued by the program whenever the line count in any page of a table exceeds the maximum set for the page type in use.

3) Line feed. This code is not accessed by the program unless it is explicitly called for by b) LINE FEED. Any other necessary line feeds are issued by the computer operating system.

4) Compressed print. A compressed print code is issued automatically by the program before a table is output (22) OUTPUT RESULTS).

5) Set normal print. A normal print code is issued automatically by the program whenever an output table is completed (22) OUTPUT RESULTS).

6) Set to standard page size. This control code has meaning on sheet feeding printers only. It is issued independently by the program as part of its initialization if LP (Laser Printer) and S (Standard Page) have been chosen as the defaults.

7) Set to legal page size. This control code has meaning on sheet feeding printers only. It is issued independently by the program as part of its initialization if LP (Laser Printer) and L (Legal Page) have been chosen as the defaults.

Examples of the dialogue in an editing session are given below. The most likely change that will be useful is the page length. It is particularly important that the compressed print, the normal print and the reset codes are correct. Most printer manuals give the correct codes.

```
#
*h

The program needs your printer device name. (eg. PRN PRN: LPT LPT: )
The current device name is - PRN
This is not a valid print device or file on your system.

CHANGE? [Y/N]: N

The program needs to know your printer type. The choices
of printer type are DM (dot matrix) or LP (laser printer).

PRINTER TYPE? [LP]: DM

The program needs to know how many lines there are on your
standard printer page.

NUMBER OF LINES? [ 60]:
```

EDITING THE PRINTER CONTROL CODES

If you chose dot matrix (DM) as the printer type, then the program will have defaulted to control codes for a Roland[DG] PR-1215 printer with continous feed paper. These codes will work with most makes of dot matrix printer. If you chose laser printer (LP) as the printer type, then the program will have defaulted to control codes for a HP Laserjet IIP printer with a sheet paper feeder. If it is necessary to make changes, then consult your printer manual to find the correct codes and enter them here.

Each code buffer has room for 32 control characters. These are entered as a string of integer numbers that represent the ASCII characters of the code sequence. Generally the first character is for carriage control and the second is the first effective character in the control or escape sequence. Note that the printer reset includes a top of form on continous feed printers and that the page size options only apply to sheet feeding printers.

```
RESET (TOP OF FORM) CODES ARE -
 43  27  64   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0
CHANGE? [N]:

PAGE EJECT CODES ARE -
  0   0   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0
CHANGE? [N]: Y

ENTER NEW CODES [i,j,k,l .... / when finished]:
43,12,/

PAGE EJECT CODES ARE -
 43  12   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0
CHANGE? [N]:

LINE FEED CODES ARE -
 43  10   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0
CHANGE? [N]:

COMPRESSED PRINT CODES ARE -
 43  15   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0
CHANGE? [N]:

NORMAL PRINT CODES ARE -
 43  18   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0   0   0   0   0   0   0   0   0
  0   0
CHANGE? [N]:
```

i) SIGNIFICANT FIGURES

This option gives allows you to change the number of significant figures in the reported wt.% of the analysis. The choices are two or three figures after the decimal.

The setting applies to both the browse and table options in 22) OUTPUT RESULTS.

The setting is saved and recalled with each formula in 3) SAVE CURRENT FORMULA and 1) CHOOSE A FORMULA.

```
*22

BROWSE?           [N]: Y
HARD COPY? [N]:
ENTER ANALYSIS NUMBERS
#? 20
#?

      Amph#2
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  23 OX                              RATIO
SIO2   37.67   6.182   SI   6.182                              Fm  .595
AL2O3  10.49   2.029   AL   1.818
TIO2    3.11    .384              8.000
CR2O3    .00    .000   AL    .211
FE2O3    .00    .000   TI    .384
FEO    18.34   2.517   CR    .000
MNO      .76    .106   FE+3  .000
MGO     6.99   1.710   FE+2 2.517
CAO    10.72   1.885   MN    .106
NA2O    2.65    .843   MG   1.710
K2O     1.78    .373              4.928
  F      .23    .119   CA   1.885
  CL     .07    .019   NA    .115
      ------  ------              2.000
TOTAL  92.81  16.167   NA    .728
      ------  ------   K     .373
TOT-O  92.70                    1.101
                       F     .119
                       CL    .019
                                  .138
PRESS ENTER TO CONTINUE:
```

```
*i

NUMBER OF SIGNIFICANT FIGURES IN THE OUTPUT? [2]: 3

*22

BROWSE?            [N]: Y
HARD COPY? [N]:
ENTER ANALYSIS NUMBERS
#? 20
#?
```

Amph#2

	WT.%	ATOMS		CALC ON	23 OX		RATIO
SIO2	37.670	6.182	SI	6.182		Fm	.595
AL2O3	10.490	2.029	AL	1.818			
TIO2	3.110	.384			8.000		
CR2O3	.000	.000	AL	.211			
FE2O3	.000	.000	TI	.384			
FEO	18.340	2.517	CR	.000			
MNO	.760	.106	FE+3	.000			
MGO	6.990	1.710	FE+2	2.517			
CAO	10.720	1.885	MN	.106			
NA2O	2.650	.843	MG	1.710			
K2O	1.780	.373			4.928		
F	.230	.119	CA	1.885			
CL	.070	.019	NA	.115			
					2.000		
TOTAL	92.810	16.167	NA	.728			
			K	.373			
TOT-O	92.697				1.101		
			F	.119			
			CL	.019			
					.138		

```
PRESS ENTER TO CONTINUE:
```

j) EDIT DEFAULT VALENCES

The disk file VALE contains default values for the valence of any element to be processed in the form of oxide components. These accessed by 2) ENTER A NEW FORMULA, 7) SPECIFY END MEMBERS and 77) LOAD FROM ASCII FILE.

```
*j

WHICH ELEMENT?: FE
VALENCE? [ 2]: 3
WHICH ELEMENT?: FE
VALENCE? [ 3]: 2
WHICH ELEMENT?: FE
VALENCE? [ 2]:
WHICH ELEMENT?: SN
VALENCE? [ 0]: 4
WHICH ELEMENT?: SN
VALENCE? [ 4]:
WHICH ELEMENT?:
```

k) DISPLAY FORMULA CODES

Prints a description of the internal details of the current formula calculation, specifically those affecting the determination of iron oxidation ratio, cation ratios and end-member components. This command compliments 5) DISPLAY CURRENT FORMULA, which is designed to present the format of the output.

F2 and F3 may appear as special element symbols in the prompts. They are used to represent Fe^{+2} and Fe^{+3} when Fe may occur in either oxidation state.

The following garnet formula will serve as an example.

Notice that the term "Element I" is defined as the element's position in the formula. A distinct position is counted for each occurrence of the element. In the present example, Ti occurs in two sites and Fe is in two forms, giving twelve items in the list of ratio codes.

Also notice that the term "Key Element I" denotes a distinct atomic species in the formula. In the table of end member codes these are mentioned in the order of their first occurrence.

Up to five ratios may be strung together as further multipliers for each key element entry in each end member.

*5

SAMPLE Garnet #2 VALUES TO BE OUTPUT

	WT.%	ATOMS	CALC ON	24 OX		WT.%	MOL.%		RATIO
SIO2	.00	.000	SI .000		Alman	.00	.00	Fmg	.000
TIO2	.00	.000	TI .000		Andra	.00	.00	.	.000
AL2O3	.00	.000		6.000	Schor	.00	.00	.	.000
CR2O3	.00	.000	TI .000		FeMel	.00	.00	.	.000
FE2O3	.00	.000	AL .000		MgMel	.00	.00	.	.000
FEO	.00	.000	CR .000		Gross	.00	.00	.	.000
MGO	.00	.000	FE+3 .000		Pyrop	.00	.00		
MNO	.00	.000	FE+2 .000		Spess	.00	.00		
CAO	.00	.000	MG .000		Uvaro	.00	.00		
	---	---		4.000		---			
TOTAL	.00	.000	FE+2 .000		TOTAL	.00			
	---	---	MG .000			---			
			MN .000						
			CA .000						
				6.000					

*k

SITE # 1 HAS:
SI TI SUBSCRIPT = 6
SITE # 2 HAS:
TI AL CR FE+3 FE+2 MG SUBSCRIPT = 4
SITE # 3 HAS:
FE+2 MG MN CA SUBSCRIPT = 6

RATIO = NUMERATOR / DENOMINATOR

WHERE: BOTH NUMERATOR AND DENOMINATOR =
SUM (MOLS ELEMENT I x COEFFICIENT)

COEFFICIENTS FOR THE NUMERATOR

Fmg	.	.	.	.	.
.0000	.0000	.0000	.0000	.0000	.0000
.0000	1.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
1.0000	.0000	1.0000	.0000	.0000	.0000
.0000	.0000	.0000	1.0000	.0000	.0000
1.0000	.0000	.0000	.0000	1.0000	.0000
.0000	.0000	.0000	.0000	.0000	1.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000

COEFFICIENTS FOR THE DENOMINATOR

Fmg	.	.	.	.	.
.0000	.0000	.0000	.0000	.0000	.0000
.0000	1.0000	.0000	.0000	.0000	.0000
.0000	1.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
1.0000	.0000	1.0000	.0000	1.0000	.0000
1.0000	.0000	.0000	1.0000	.0000	1.0000
1.0000	.0000	1.0000	.0000	1.0000	.0000
1.0000	.0000	.0000	1.0000	.0000	1.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000

END MEMBER WT.% =
(ITERATION OF [SUM (MOLS KEY ELEMENT I x MULTIPLIER x RATIOS)])
x MOLECULAR WEIGHT

END MEMBER MOLECULAR WEIGHTS

Alman	Andra	Schor	FeMel	MgMel	Gross	Pyrop	Spess	Uvaro
995.56	1016.42	1135.28	1000.52	937.44	900.94	806.32	990.10	1001.02

END MEMBER MULTIPLIERS
END MEMBER RATIO VECTORS

	Alman	Andra	Schor	FeMel	MgMel	Gross	Pyrop	Spess	Uvaro
SI	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
TI	.0000	-.1667	.1667	.0000	.0000	-.1667	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
AL	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
CR	.0000	.0000	.0000	.0000	.0000	-.2500	.0000	.0000	.2500
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
F3	.0000	.2500	.0000	.0000	.0000	-.2500	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
F2	.1667	.0000	-.1667	.5000	.0000	-.5000	.0000	.0000	.0000
	16 0	0 0	4 0	4 0	0 0	4 0	0 0	0 0	0 0
MG	.0000	.0000	-.1667	.0000	.5000	-.5000	.1667	.0000	.0000
	0 0	0 0	8 0	0 0	8 0	8 0	32 0	0 0	0 0
MN	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.1667	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
CA	.0000	.0000	.0000	.0000	.0000	.1667	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0

RATIO VECTOR	MEANS MULTIPLY BY RATIOS
16 0	0 0 0 0 5 0
4 0	0 0 3 0 0 0
8 0	0 0 0 4 0 0
32 0	0 0 0 0 0 6

l) EDIT END MEMBER CODES

Provides an opportunity to over-write the multipliers (codes) that the program uses to calculate the defined end members.

In the garnet example used above for k) DISPLAY END MEMBER CODES, the Andradite (Andra) component is based on F3 as the key element which overestimates the amount of Andradite because in part, it is included in the Schorlomite or Ti end member. This is compensated for by entering a negative weight for Ti in the Andradite summation. If ratio number two were an adequate expression of the division of F3 between Andradite and Schorlomite, then it could be used as an alternative means of compensation.

```
*l

END MEMBER?: Andra
Andra    MOLECULAR WT. [ 1016.42]?:
ELEMENT NUMBER?: 2
MULTIPLIER =   -.1667
CHANGE? [N]: y
VALUE?: 0.0000
NO RATIO MULTIPLIERS
CHANGE? [N]:
FINISHED? [N]:
END MEMBER?: Andra
Andra    MOLECULAR WT. [ 1016.42]?:
ELEMENT NUMBER?: 5
MULTIPLIER =    .2500
CHANGE? [N]:
NO RATIO MULTIPLIERS
CHANGE? [N]: y
WHICH RATIOS?: 2
FINISHED? [N]: Y

*k

SITE #  1 HAS:
SI TI  SUBSCRIPT =   6
SITE #  2 HAS:
TI AL CR FE+3 FE+2 MG  SUBSCRIPT =   4
SITE #  3 HAS:
FE+2 MG MN CA  SUBSCRIPT =   6
```

RATIO = NUMERATOR / DENOMINATOR

WHERE: BOTH NUMERATOR AND DENOMINATOR =
SUM (MOLS ELEMENT I x CODE)

COEFFICIENTS FOR THE NUMERATOR

Fmg	.	.	.	.	.
.0000	.0000	.0000	.0000	.0000	.0000
.0000	1.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
1.0000	.0000	1.0000	.0000	.0000	.0000
.0000	.0000	.0000	1.0000	.0000	.0000
1.0000	.0000	.0000	.0000	1.0000	.0000
.0000	.0000	.0000	.0000	.0000	1.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000

COEFFICIENTS FOR THE DENOMINATOR

Fmg	.	.	.	.	.
.0000	.0000	.0000	.0000	.0000	.0000
.0000	1.0000	.0000	.0000	.0000	.0000
.0000	1.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000
1.0000	.0000	1.0000	.0000	1.0000	.0000
1.0000	.0000	.0000	1.0000	.0000	1.0000
1.0000	.0000	1.0000	.0000	1.0000	.0000
1.0000	.0000	.0000	1.0000	.0000	1.0000
.0000	.0000	.0000	.0000	.0000	.0000
.0000	.0000	.0000	.0000	.0000	.0000

END MEMBER WT.% =
(ITERATION OF [SUM (MOLS KEY ELEMENT I x MULTIPLIER x RATIOS)])
x MOLECULAR WEIGHT

END MEMBER MOLECULAR WEIGHTS

Alman	Andra	Schor	FeMel	MgMel	Gross	Pyrop	Spess	Uvaro
995.56	1016.42	1135.28	1000.52	937.44	900.94	806.32	990.10	1001.02

END MEMBER MULTIPLIERS
END MEMBER RATIO VECTORS

	Alman	Andra	Schor	FeMel	MgMel	Gross	Pyrop	Spess	Uvaro
SI	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
TI	.0000	.0000	.1667	.0000	.0000	-.1667	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
AL	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
CR	.0000	.0000	.0000	.0000	.0000	-.2500	.0000	.0000	.2500
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
F3	.0000	.2500	.0000	.0000	.0000	-.2500	.0000	.0000	.0000
	0 0	2 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
F2	.1667	.0000	-.1667	.5000	.0000	-.5000	.0000	.0000	.0000
	16 0	0 0	4 0	4 0	0 0	4 0	0 0	0 0	0 0
MG	.0000	.0000	-.1667	.0000	.5000	-.5000	.1667	.0000	.0000
	0 0	0 0	8 0	0 0	8 0	8 0	32 0	0 0	0 0
MN	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.1667	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
CA	.0000	.0000	.0000	.0000	.0000	.1667	.0000	.0000	.0000
	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0

RATIO VECTOR	MEANS MULTIPLY BY RATIOS
2 0	0 2 0 0 0 0
16 0	0 0 0 0 5 0
4 0	0 0 3 0 0 0
8 0	0 0 0 4 0 0
32 0	0 0 0 0 0 6

m) EDIT RATIO CODES

Provides an opportunity to over-write the multipliers (codes) that the program uses to calculate the defined ratios.

In the garnet example used above for k) DISPLAY END MEMBER CODES, Fmg has already been defined as (Total Fe)/(Total Fe + Total Mg). The steps below will redefine the ratio as (Total Fe)/(Total Fe + Total Mg + Mn).

```
*m

RATIO NUMBER? : 1

THE CODES FOR RATIO #  1 (  Fmg) ARE ...

                            NUMERATOR

   SI      TI      TI      AL      CR      F3      F2      MG      F2      MG
  .0000   .0000   .0000   .0000   .0000   .0000  1.0000   .0000  1.0000   .0000

   MN      CA
  .0000   .0000
                            DENOMINATOR

   SI      TI      TI      AL      CR      F3      F2      MG      F2      MG
  .0000   .0000   .0000   .0000   .0000   .0000  1.0000  1.0000  1.0000  1.0000

   MN      CA
  .0000   .0000

CHANGE? [N]: Y
NUMERATOR OR DENOMINATOR? N/D: D
ELEMENT NUMBER?: 11
CODE    .0000
CHANGE? [N]: Y
VALUE?: 1.0000
FINISHED? [N]: Y

*m

THE CODES FOR RATIO #  1 (  Fmg) ARE ...

                            NUMERATOR

   SI      TI      TI      AL      CR      F3      F2      MG      F2      MG
  .0000   .0000   .0000   .0000   .0000   .0000  1.0000   .0000  1.0000   .0000

   MN      CA
  .0000   .0000
                            DENOMINATOR

   SI      TI      TI      AL      CR      F3      F2      MG      F2      MG
  .0000   .0000   .0000   .0000   .0000   .0000  1.0000  1.0000  1.0000  1.0000

   MN      CA
 1.0000   .0000

CHANGE? [N]:
FINISHED? [N]: Y
```

p) PRINT FORMULA DIRECTORY

Prints a hard copy directory of the output formulae that have been saved in the currently specified formula directory.

See 99) CHANGE FORMULA DIRECTORY and 1) CHOOSE A FORMULA.

r) RETURN TO MAIN MENU

0) EXIT PROGRAM

11) ANALYSIS DIRECTORY

Displays a directory of the labels of any analyses that are in the working data buffer. The buffer has a capacity of 500 analyses. The labels are eight characters each, consequently a standard monitor can only display 100 labels at one time. For convenience the directory is divided into five pages, numbered from 0 to 4. In this way analyses 0 to 100 are displayed on page 0, analyses 101 to 200 are displayed on page 1, ...etc....

See also 00) CHANGE ANALYSIS DIRECTORY.

```
*11

WHICH PAGE? (0-4) : 1
                      STORED ANALYSES (USER)  (PAGE 1)                    (DIR)
 101      102      103      104      105      106      107      108      109      110
05P4002705S4002805P5002905S5003005C40031     0001     0002     0003     0004     000
 111      112      113      114      115      116      117      118      119      120
    0006GT-80007GT-90008GT-10009HB-10010HB-10011PL-10012    0013GT-10014PL-1001
 121      122      123      124      125      126      127      128      129      130
PX-10016HB-10017
 131      132      133      134      135      136      137      138      139      140

 141      142      143      144      145      146      147      148      149      150

 151      152      153      154      155      156      157      158      159      160

 161      162      163      164      165      166      167      168      169      170

 171      172      173      174      175      176      177      178      179      180

 181      182      183      184      185      186      187      188      189      190

 191      192      193      194      195      196      197      198      199      200

HARD COPY? [N]: Y
```

The labels in this display are not spaced and the final character of every tenth label is missing because standard monitors are limited to 79 characters per line. The directory is more readable if it is printed as hard copy -

```
          STORED ANALYSES (USER)  (PAGE 1)                    (DIR)

101       102       103       104       105       106       107       108       109       110
05P40027 05S40028 05P50029 05S50030 05C40031      0001      0002      0003      0004      0005
111       112       113       114       115       116       117       118       119       120
     0006 GT-80007 GT-90008 GT-10009 HB-10010 HB-10011 PL-10012      0013 GT-10014 PL-10015
121       122       123       124       125       126       127       128       129       130
PX-10016 HB-10017
131       132       133       134       135       136       137       138       139       140

141       142       143       144       145       146       147       148       149       150

151       152       153       154       155       156       157       158       159       160

161       162       163       164       165       166       167       168       169       170

171       172       173       174       175       176       177       178       179       180

181       182       183       184       185       186       187       188       189       190

191       192       193       194       195       196       197       198       199       200
```

The program can access multiple working data buffers by using passwords (00) CHANGE ANALYSIS DIRECTORY). Each working data buffer consists of two disk files (Appendix A) that contain a copy of up to 500 analyses in raw form (55) PRINT RAW DATA). The program can import data into the current working data buffer (77) LOAD FROM ASCII FILE) if the data is in a text file that conforms to the format in Appendix D.

22) OUTPUT RESULTS

Produce the finished table of results. Includes a browse option which displays the finished result one analyses at a time.

The format and items to be included are controlled by the choice of formula (1) CHOOSE A FORMULA). There are ten analyses printed per page of the table.

Analyses are selected for inclusion in the table by directory number (11) ANALYSIS DIRECTORY) and in any order or as any subset. There is also provision to call for analyses to be included in the table by a wildcard search of the labels. If there is no change in formula, a number of tables may be specified before any are printed. See Chapter 3-3 on analysis numbering and the designation of data subsets.

Other command options include: a) comments as table headers, b) append average and standard deviation, c) print average and standard deviation only, d) exclude formula, e) number of copies and f) choose destination of printer and/or disk file.

The standard deviation is calculated as ...

$$SD = \frac{\sqrt{\sum (v_i - avg)^2}}{n-1}$$

Where ... v_i = the i^{th} item in the list and

n = number of items

Caution: There will be numerical inconsistencies when averages are calculated and stoichiometric iron is calculated. The variance is in the iron values only. They arise because the iron is divided after the iron average is prepared.

Each table that is printed is automatically saved in ASCII form in the file named DUMP. DUMP always contains a copy of the last table printed. There is an option to suppress the hard copy if you choose to send the data to a file other than DUMP. There is also an option to append or overwrite when a duplicate filename is given.

The table is in column orientation which is not easily imported into spreadsheets or databases. A separate utility program called CONVTAB has been provided to deal with this problem. It will convert tables produced by MR into row orientation. CONVTAB has instructions that are displayed at runtime.

```
*77

ENTER THE FULL PATHNAME FOR THE DATA TO BE LOADED
?: amphibole.dat
APPEND TO PREVIOUSLY LOADED ANALYSES? [N]:


*11

WHICH PAGE? (0-4) :
                    STORED ANALYSES (GSC1)  (PAGE 0)                    (DIR)
   1       2       3       4       5       6       7       8       9      10
KARSTD     2       3       4       5       6       7       8       9      10
  11      12      13      14      15      16      17      18      19      20

  21      22      23      24      25      26      27      28      29      30

  31      32      33      34      35      36      37      38      39      40

  41      42      43      44      45      46      47      48      49      50

  51      52      53      54      55      56      57      58      59      60

  61      62      63      64      65      66      67      68      69      70

  71      72      73      74      75      76      77      78      79      80

  81      82      83      84      85      86      87      88      89      90

  91      92      93      94      95      96      97      98      99     100

HARD COPY? [N]:


*1

                    STORED FORMULAE (DOCU)

  1 Feldspar        2 Feldspar #1     3 Feldspar #2     4 Feldspar #3
  5 Feldspar #4     6 Feldspar #5     7 Colusite #1     8 Colusite #2
  9 Chalcopyr #1   10 Chalcopyr #2   11 Scapolite #1   12 Scapolte #2
 13 Sodalite #1    14 Sodalite #2    15 Analcime #1    16 Analcime #2
 17 Phlogopite #1  18 Phlogopite #2  19 Phlogopite #3  20 Garnet #1
 21 Serpentine #1  22 Serpentine #2  23 Serpentine #3  24 Chromite #1
 25 Amphibole #1   26 Amphibole #2   27 Amphibole #3   28 Amphibole #4
 29 Amphibole #5   30 Smectite #1    31 Smectite #2    32 Smectite #3
 33 Tourmaline #1  34 Tourmaline #2

RECALL WHICH FORMULA?: 29
```

```
    SAMPLE    Amphibole        VALUES TO BE OUTPUT
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  23 OX                                  RATIO
SIO2     .00    .000   SI    .000                                Fm  .000
AL2O3    .00    .000   AL    .000
TIO2     .00    .000               8.000
CR2O3    .00    .000   AL    .000
FE2O3    .00    .000   TI    .000
FEO      .00    .000   CR    .000
MNO      .00    .000   FE+3  .000
MGO      .00    .000   FE+2  .000
CAO      .00    .000   MN    .000
NA2O     .00    .000   MG    .000
K2O      .00    .000               5.000
  F      .00    .000   CA    .000
  CL     .00    .000   NA    .000
       ------  ------               2.000
TOTAL    .00    .000   NA    .000
       ------  ------   K     .000
TOT-O    .00                       1.000
                        F     .000
                        CL    .000
                                   2.000
PRESS ENTER FOR THE MENU:


*22


BROWSE?            [N]: Y
HARD COPY? [N]:
ENTER ANALYSIS NUMBERS
#? 1
#?


      KARSTD
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON  23 OX                                  RATIO
SIO2    37.67   6.181   SI   6.181                                Fm  .595
AL2O3   10.49   2.029   AL   1.819
TIO2     3.11    .384               8.000
CR2O3     .00    .000   AL    .210
FE2O3     .00    .000   TI    .384
FEO     18.34   2.517   CR    .000
MNO       .76    .106   FE+3  .000
MGO      6.99   1.710   FE+2 2.517
CAO     10.72   1.885   MN    .106
NA2O     2.65    .843   MG   1.710
K2O      1.78    .373               4.927
  F       .23    .119   CA   1.885
  CL      .07    .019   NA    .115
       ------  ------               2.000
TOTAL   92.81  16.166   NA    .728
       ------  ------   K     .373
TOT-O   92.70                       1.101
                        F     .119
                        CL    .019
                                    .138
PRESS ENTER TO CONTINUE:
```

```
*22

AVERAGE?           [N]: Y
AVERAGE ONLY?      [N]:
PRINT FORMULA?     [Y]:
ENTER # OF COPIES  [1]:
COPY TO?        [DUMP]: amphibol.tab
HARD COPY? [N]:
ENTER A HEADING?   [N]:
ENTER ANALYSIS NUMBERS
#? 1
#? -4
#?
```

	KARSTD	2	3	4	AVERAGE	SD
SIO2	37.67	37.71	37.23	37.18	37.45	.28
AL2O3	10.49	10.82	10.63	11.18	10.78	.30
TIO2	3.11	4.16	4.08	3.14	3.62	.58
CR2O3	.00	.06	.03	.04	.03	.03
FE2O3	.00	.62	.29	2.90	.44	1.32
FEO	18.34	20.07	20.11	19.64	20.00	.83
MNO	.76	.63	.66	.98	.76	.16
MGO	6.99	6.98	6.94	5.85	6.69	.56
CAO	10.72	10.77	10.74	10.25	10.62	.25
NA2O	2.65	2.83	2.82	2.82	2.78	.09
K2O	1.78	1.88	1.91	2.00	1.89	.09
F	.23	.04	.16	.03	.12	.10
CL	.07	.06	.08	.04	.06	.02
TOTAL	92.81	96.63	95.68	96.05	95.24	1.70
TOT-O	92.70	96.60	95.59	96.03	95.18	1.74
			FORMULA (BASIS 23 OXYGEN(S))			
SI	6.182	5.990	5.991	5.974	6.042	.099
AL	1.818	2.010	2.009	2.026	1.958	.099
	8.000	8.000	8.000	8.000	8.000	.000
AL	.211	.016	.007	.091	.092	.094
TI	.384	.497	.494	.379	.440	.066
CR	.000	.008	.004	.005	.004	.003
FE+3	.000	.074	.035	.351	.053	.160
FE+2	2.517	2.666	2.706	2.639	2.699	.081
MN	.106	.085	.090	.133	.104	.022
MG	1.710	1.653	1.665	1.401	1.609	.140
	4.928	4.999	5.001	4.999	5.001	.036
CA	1.885	1.833	1.852	1.765	1.836	.051
NA	.115	.167	.148	.235	.164	.051
	2.000	2.000	2.000	2.000	2.000	.000
NA	.728	.705	.732	.644	.706	.041
K	.373	.381	.392	.410	.390	.016
	1.101	1.086	1.124	1.054	1.096	.029
F	.119	.020	.081	.015	.059	.050
CL	.019	.016	.022	.011	.017	.005
	.138	.036	.103	.026	.076	.054
Fm	.595	.624	.622	.681	.631	.036

33) ENTER WT.%

Provides for keyboard entry of analyses into the working data buffer. There must be a current formula (1) CHOOSE A FORMULA) to provide the list of elements in the analysis being entered. If the current formula is in oxide format (2) ENTER A NEW FORMULA), then you have the choice of entering the data as wt.% element or wt.% oxide.

F2 and F3 may appear as special element symbols in the prompts. They are used to represent Fe^{+2} and Fe^{+3} when Fe may occur in either oxidation state.

If a blank label is given, then "+" is inserted by the program as a placeholder.

See also 00) CHANGE ANALYSIS DIRECTORY.

Using a three element current formula in non-oxide format .....

```
*1

                STORED FORMULAE (DOCU)

  1 Feldspar        2 Feldspar #1     3 Feldspar #2     4 Feldspar #3
  5 Feldspar #4     6 Feldspar #5     7 Colusite #1     8 Colusite #2
  9 Chalcopyr #1   10 Chalcopyr #2   11 Scapolite #1   12 Scapolte #2
 13 Sodalite #1    14 Sodalite #2    15 Analcime #1    16 Analcime #2
 17 Phlogopite #1  18 Phlogopite #2  19 Phlogopite #3  20 Garnet #1
 21 Serpentine #1  22 Serpentine #2  23 Serpentine #3  24 Chromite #1
 25 Amphibole #1   26 Amphibole #2   27 Amphibole #3   28 Amphibole #4
 29 Amphibole #5   30 Smectite #1    31 Smectite #2    32 Smectite #3
 33 Tourmaline #1  34 Tourmaline #2

RECALL WHICH FORMULA?: 9

*33

LABEL?: CuFeS2
ENTER WT.% ELEMENTS   (Include decimal)
   CU?:34.54
   FE?:30.66
   S ?:35.02
      CuFeS2
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   4 AT
  CU   34.54    .995
  FE   30.66   1.005
  S    35.02   2.000
      ------  ------
TOTAL 100.22   4.000
      ------  ------

HARD COPY? [N]:
SAVE? [N]: Y
#  1  SAVED AS : CuFeS2
FINISHED? [N]: Y
```

Using a six element current formula in oxide format .....

```
*1

                  STORED FORMULAE (DOCU)

  1 Feldspar        2 Feldspar #1     3 Feldspar #2     4 Feldspar #3
  5 Feldspar #4     6 Feldspar #5     7 Colusite #1     8 Colusite #2
  9 Chalcopyr #1   10 Chalcopyr #2   11 Scapolite #1   12 Scapolte #2
 13 Sodalite #1    14 Sodalite #2    15 Analcime #1    16 Analcime #2
 17 Phlogopite #1  18 Phlogopite #2  19 Phlogopite #3  20 Garnet #1
 21 Serpentine #1  22 Serpentine #2  23 Serpentine #3  24 Chromite #1
 25 Amphibole #1   26 Amphibole #2   27 Amphibole #3   28 Amphibole #4
 29 Amphibole #5   30 Smectite #1    31 Smectite #2    32 Smectite #3
 33 Tourmaline #1  34 Tourmaline #2

RECALL WHICH FORMULA?: 6


*33


ENTER AS % OXIDES? [N]: Y
LABEL?: Orthocl
ENTER WT.% OXIDES     (Include decimal)
SIO2 ?:64.84
AL2O3?:17.42
NA2O ?:.78
CAO  ?:
K2O  ?:15.25
FEO  ?:.98
      Orthocl
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   8 OX
SIO2   64.84   3.020
AL2O3  17.42    .956
NA2O     .78    .070
CAO      .00    .000
K2O    15.25    .906
FEO      .98    .038
      ------  ------
TOTAL  99.27   4.990
      ------  ------

HARD COPY? [N]:
SAVE? [N]: Y
#  2  SAVED AS : Orthocl
FINISHED? [N]: Y
```

44) EDIT ANALYSES

Provides an opportunity to change labels or values for analyses in the working data buffer. The ability to change labels is particularly useful if you intend to use the wildcard system of selecting data subsets for processing (Chapter 3-3).

This option is also useful for browsing through the working data buffer without resorting to hard copy.

F2 and F3 may appear as special element symbols in the prompts. They are used to represent Fe^{+2} and Fe^{+3} when Fe may occur in either oxidation state.

See also 11) ANALYSIS DIRECTORY , 77) LOAD FROM ASCII FILE and 00) CHANGE ANALYSIS DIRECTORY.

```
*44

ENTER ANALYSIS NUMBERS
#? 1
#? 2
#?

  1: [KARSTD  ]?
   O       SI      AL      TI      CR      F3      F2      MN      MG      CA
.37321  .17608  .05552  .01864  .00000  .00000  .14256  .00589  .04216  .07662
  NA       K       F       C
.01966  .01478  .00230  .00070
--------------------------------------------------------------------------------

CHANGE? [N]: Y
WEIGHT FRACTION O : [ .37321]?
WEIGHT FRACTION SI: [ .17608]?
WEIGHT FRACTION AL: [ .05552]?
WEIGHT FRACTION TI: [ .01864]?
WEIGHT FRACTION CR: [ .00000]?
WEIGHT FRACTION F3: [ .00000]? .07128
WEIGHT FRACTION F2: [ .14256]? .07128
WEIGHT FRACTION MN: [ .00589]?
WEIGHT FRACTION MG: [ .04216]?
WEIGHT FRACTION CA: [ .07662]?
WEIGHT FRACTION NA: [ .01966]?
WEIGHT FRACTION K : [ .01478]?
WEIGHT FRACTION F : [ .00230]?
WEIGHT FRACTION CL: [ .00070]?
```

```
  2: [  2     ]? KARSTD
   O       SI      AL      TI      CR      F3      F2      MN      MG      CA
.38553  .17627  .05726  .02494  .00041  .00434  .15601  .00488  .04210  .07697
  NA       K       F      CL
.02099  .01561  .00040  .00060
--------------------------------------------------------------------------------

CHANGE? [N]:


*44

ENTER ANALYSIS NUMBERS
#? 1
#? 2
#?

  1: [KARSTD  ]?
   O       SI      AL      TI      CR      F3      F2      MN      MG      CA
.37321  .17608  .05552  .01864  .00000  .07128  .07128  .00589  .04216  .07662
  NA       K       F      CL
.01966  .01478  .00230  .00070
--------------------------------------------------------------------------------

CHANGE? [N]:

  2: [KARSTD  ]?
   O       SI      AL      TI      CR      F3      F2      MN      MG      CA
.38553  .17627  .05726  .02494  .00041  .00434  .15601  .00488  .04210  .07697
  NA       K       F      CL
.02099  .01561  .00040  .00060
--------------------------------------------------------------------------------

CHANGE? [N]:
```

55) PRINT RAW DATA

Prints a subset of data from the working data buffer. The data is not processed in any way and is printed exactly as it occurs in the buffer. This command is useful when you are simply looking through the data that has been loaded in the buffer. You may use 22) OUTPUT RESULTS or 44) EDIT ANALYSES to browse through the working data buffer without resorting to hard copy.

F2 and F3 may appear as special symbols in the element lists. They are used to represent Fe^{+2} and Fe^{+3} when Fe may occur in either oxidation state.

See also 11) ANALYSIS DIRECTORY , 77) LOAD FROM ASCII FILE and 00) CHANGE ANALYSIS DIRECTORY.

See Chapter 3-3 on analysis numbering and the designation of data subsets.

```
*55

ENTER ANALYSIS NUMBERS
#? 1
#? -5
#?


   1:  92-9-6-4
    O       NA      K       SI      FE      AL      CA      BA      SR
  .47804  .04294  .00330  .26344  .00037  .14959  .07263  .00117  .00005
-------------------------------------------------------------------------------
   2:  92-9-6-5
    O       NA      K       SI      FE      AL      CA      BA      SR
  .47719  .04063  .00295  .25952  .00136  .15231  .07734  .00000  .00030
-------------------------------------------------------------------------------
   3:  92-9-6-6
    O       NA      K       SI      FE      AL      CA      BA      SR
  .47713  .04387  .00368  .26446  .00068  .14769  .07017  .00144  .00051
-------------------------------------------------------------------------------
   4:  92-9-6-D
    O       NA      K       SI      FE      AL      CA      BA      SR
  .47780  .03963  .00351  .26139  .00100  .15191  .07540  .00000  .00000
-------------------------------------------------------------------------------
   5:  92-9-6-E
    O       NA      K       SI      FE      AL      CA      BA      SR
  .45783  .00260  .13326  .29559  .00027  .10045  .00487  .01128  .00127
-------------------------------------------------------------------------------
```

66) DELETE ANALYSES

Deletes an analysis or a subset of analyses from the working data buffer. You have the option of packing the analysis storage to remove any "holes" in the data set remaining in the buffer. If the "append" option is chosen in 77) LOAD FROM ASCII FILE or if new analyses are entered by 33) ENTER WT.% then the new data will be added to the data set by filling the blanks first.

Any "holes" already in the data set in the working data buffer may be removed by selecting them for deletion and choosing the pack option.

See also 11) ANALYSIS DIRECTORY and 00) CHANGE ANALYSIS DIRECTORY.

See Chapter 3-3 on analysis numbering and the designation of data subsets.

```
*11

WHICH PAGE? (0-4) :
                    STORED ANALYSES (    ) (PAGE 0)                  (DIR)
   1       2       3       4       5       6       7       8       9      10
PL90B1R PL90B1C PL90B2R PL90B2C OL90B3R PL90B3R PL90B3C PL95B1R PL95B1C KS95B1R
  11      12      13      14      15      16      17      18      19      20
KS95B1C KS95B2R KS95B1C PL95B2R PL95B2C KS95B3R KS95B3C PL95B3R PL95B3C PL1051R
  21      22      23      24      25      26      27      28      29      30
PL1051C PL1052R PL1052C KS1051R KS1051C KS1052R KS1052C PL1053R PL1053C KS1053R
  31      32      33      34      35      36      37      38      39      40
KS1053C OL931R  OL90B1C OL90B2R OL90B2C OP90B1R OP90B1C CP90B1R CP90B1C CP90B2R
  41      42      43      44      45      46      47      48      49      50
CP90B2C IL90B1R IL90B1C OL90B3R OL90B3C OP90B3R OP90B3C IL90B2R IL90B2C CP90B3R
  51      52      53      54      55      56      57      58      59      60
CP90B3C MT90B1R MT90B1C CP95B1R CP95B1C OP95B1R OP95B1C CP95B2R CP95B2C OP95B2R
  61      62      63      64      65      66      67      68      69      70
OP95B2C IL95B1R IL95B1C MT95B1R MT95B1C IL95B2R IL95B2C MT95B2R MT95B2C OP95B3R
  71      72      73      74      75      76      77      78      79      80
OP95B3C CP95B3R CP95B3C MT95B3R MT95B3C IL95B3R IL95B3C CP1051R CP1051C MT1051R
  81      82      83      84      85      86      87      88      89      90
MT1051C IL1051R IL1051C CP1052R CP1052C MT1052R MT1052C IL1052R IL1052C CPX1053
  91      92      93      94      95      96      97      98      99     100
CPX1053CCP1054R CP1054C MT1053R MT1053C IL1053R IL1053C
HARD COPY? [N]:
```

```
*66

ENTER ANALYSIS NUMBERS
#? *
ENTER WILDCARDED LABEL TO BE USED (8 char.): OL******
#? *
ENTER WILDCARDED LABEL TO BE USED (8 char.): MT******
#? *
ENTER WILDCARDED LABEL TO BE USED (8 char.): IL******
#?
PACK ANALYSIS STORAGE? [Y]:


                    WAIT: PACKING ANALYSIS STORAGE


*11

WHICH PAGE? (0-4) :
                        STORED ANALYSES. (     ) (PAGE 0)                    (DIR)
   1       2       3       4       5       6       7       8       9       10
PL90B1R PL90B1C PL90B2R PL90B2C PL90B3R PL90B3C PL95B1R PL95B1C KS95B1R KS95B1C
  11      12      13      14      15      16      17      18      19      20
KS95B2R KS95B1C PL95B2R PL95B2C KS95B3R KS95B3C PL95B3R PL95B3C PL1051R PL1051C
  21      22      23      24      25      26      27      28      29      30
PL1052R PL1052C KS1051R KS1051C KS1052R KS1052C PL1053R PL1053C KS1053R KS1053C
  31      32      33      34      35      36      37      38      39      40
OP90B1R OP90B1C CP90B1R CP90B1C CP90B2R CP90B2C OP90B3R OP90B3C CP90B3R CP90B3C
  41      42      43      44      45      46      47      48      49      50
CP95B1R CP95B1C OP95B1R OP95B1C CP95B2R CP95B2C OP95B2R OP95B2C OP95B3R OP95B3C
  51      52      53      54      55      56      57      58      59      60
CP95B3R CP95B3C CP1051R CP1051C CP1052R CP1052C CPX1053RCPX1053CCP1054R CP1054C
  61      62      63      64      65      66      67      68      69      70

  71      72      73      74      75      76      77      78      79      80

  81      82      83      84      85      86      87      88      89      90

  91      92      93      94      95      96      97      98      99     100

HARD COPY? [N]:
```

77) LOAD FROM ASCII FILE

Imports data into the working data buffer if it is in a text file that conforms to the format described in Appendix D.

You may choose to overwrite any existing data starting with position number one in the working data buffer. This is the most frequently chosen option since the relation between analysis numbering and buffer position numbering is maintained (ie. Analysis number one in the data set is in position number one in the buffer).

You may also choose to append to any existing data. In this case the working data buffer is filled starting with the first blank and filling successive blanks in order. Only blanks are filled and no data is overwritten.

If there is a blank label in the incoming data set, then the analyses is not loaded.

See also 11) ANALYSIS DIRECTORY and 66) DELETE ANALYSES.

88) WRITE TO ASCII FILE

Writes analytical data to a disk file in the ASCII format described in Appendix D. These files may in turn be reloaded into the working data buffer (77) LOAD FROM ASCII FILE).

The structure of the output is controlled by the current formula and keyboard selection of the data subset. See 1) CHOOSE A FORMULA on formula selection and Chapter 3-3 on analysis numbering and the designation of data subsets. These features allow you to exclude elements, change element order, exclude analyses and change analysis order.

There is an option to append an average or output the average only. There is also an option to append to an already existing output file. This provides a means of collating a file of averages.

There is also an option to exclude the final comma from each data record. This is to improve compatibility with some other database, spreadsheet and mineral data programs that are in general use (eg. MINPET). The toggle on this option remains set until changed, even after restarting the program.

```
*11

WHICH PAGE? (0-4) :
                        STORED ANALYSES (GSC2)  (PAGE 0)                  (DIR)
   1       2       3       4       5       6       7       8       9       10
KARSTD     2       3       4       5       6       7       8       9       10
  11      12      13      14      15      16      17      18      19      20

  21      22      23      24      25      26      27      28      29      30

  31      32      33      34      35      36      37      38      39      40

  41      42      43      44      45      46      47      48      49      50

  51      52      53      54      55      56      57      58      59      60

  61      62      63      64      65      66      67      68      69      70

  71      72      73      74      75      76      77      78      79      80

  81      82      83      84      85      86      87      88      89      90

  91      92      93      94      95      96      97      98      99     100

HARD COPY? [N]:


*44

ENTER ANALYSIS NUMBERS
#? 1
#? 5
#?


  1: [KARSTD  ]?
   O       SI      AL      TI      CR      F3      F2      MN      MG      CA
 .37321  .17608  .05552  .01864  .00000  .00000  .14256  .00589  .04216  .07662
   NA      K       F       CL
 .01966  .01478  .00230  .00070
--------------------------------------------------------------------------------

CHANGE? [N]:


  5: [  5     ]?
   O       SI      AL      TI      CR      F3      F2      MN      MG      CA
 .38447  .17674  .05869  .02392  .00034  .00000  .15717  .00612  .04071  .07762
   NA      K       F       CL
 .01996  .01577  .00020  .00060
--------------------------------------------------------------------------------

CHANGE? [N]:
```

```
*2

MINERAL NAME? :Silicate
FORMULA? :Si,Al,Na,Ca,K,Fe,O
CALCULATE AS OXIDES? [Y]:
DIVIDE THE FORMULA INTO SITES? [Y]: N
USE OXYGEN TO SCALE THE CALCULATED FORMULA? [Y]:
SPECIFY RATIOS?      [Y\N]: N
SPECIFY END MEMBERS? [Y\N]: N


    SAMPLE    Silicate         VALUES TO BE OUTPUT
-------------------------------------------------------------------------------
        WT.%   ATOMS     CALC ON   1 OX
NA2O     .00    .000
MGO      .00    .000
AL2O3    .00    .000
SIO2     .00    .000
K2O      .00    .000
CAO      .00    .000
TIO2     .00    .000
CR2O3    .00    .000
MNO      .00    .000
FEO      .00    .000
      ------  ------
TOTAL    .00    .000
      ------  ------

SAVE THIS FORMULA? [N]: Y
FORMULA IS NAMED Silicate
CHANGE? [N]:


*88

AVERAGE?          [N]: Y
AVERAGE ONLY?     [N]: Y
ENTER THE FULL PATHNAME OF THE DESTINATION ASCII FILE:
: average.dat
USE COMMA TO END RECORDS? [Y]:
ENTER ANALYSIS NUMBERS
#? 1
#? -10
#?


                    WAIT: DOWNLOADING ANALYSES


CALCULATING STANDARD DEVIATIONS
ENTER LABEL: avg
```

```
*77

ENTER THE FULL PATHNAME FOR THE DATA TO BE LOADED
?: average.dat
APPEND TO PREVIOUSLY LOADED ANALYSES? [N]: Y

                        WAIT: TRANSFERRING DATA TO MR

*11

WHICH PAGE? (0-4) :
                        STORED ANALYSES (    ) (PAGE 0)                  (DIR)
   1       2       3       4       5       6       7       8       9       10
KARSTD     2       3       4       5       6       7       8       9       10
  11      12      13      14      15      16      17      18      19      20
avg
  21      22      23      24      25      26      27      28      29      30

  31      32      33      34      35      36      37      38      39      40

  41      42      43      44      45      46      47      48      49      50

  51      52      53      54      55      56      57      58      59      60

  61      62      63      64      65      66      67      68      69      70

  71      72      73      74      75      76      77      78      79      80

  81      82      83      84      85      86      87      88      89      90

  91      92      93      94      95      96      97      98      99     100

HARD COPY? [N]:


*44

ENTER ANALYSIS NUMBERS
#? 1
#? 11
#?

  1: [KARSTD  ?]
 O       SI      AL      TI      CR      F3      F2      MN      MG      CA
 .3732   .1761   .0555   .0186   .0000   .0000   .1426   .0059   .0422   .0766
 NA      K       F       CL
 .0197   .0148   .0023   .0007
--------------------------------------------------------------------------------

CHANGE? [N]:


 11: [avg      ?]
 O       NA      MG      AL      SI      K       CA      TI      CR      MN
 .3813   .0206   .0395   .0590   .1753   .0158   .0763   .0210   .0001   .0062
 FE
 .1620
--------------------------------------------------------------------------------

CHANGE? [N]:
```

99) CHANGE FORMULA DIRECTORY

Changes the directory of stored formulae to be accessed by 1) CHOOSE A FORMULA , 3) SAVE CURRENT FORMULA and 4) DELETE FORMULA.

Provision has been made for multiple directories of stored formulae where each directory has a capacity of 100 definitions and a four character password. The password of the active formula directory is shown in brackets in the title line of its displayed directory.

The formula directory password is always set to the default (GSC1) at run-time. The installation copy of the program contains a set of frequently used formulae in the default directory. The examples used in this documentation are included in the installation copy under the password DOCU. See Appendix A for details on how to change any passworded directory into the default (GSC1) directory.

There is no command in the program that will reveal the number of formula directories that have been created and their passwords. See Appendix A for details on how to obtain this information from the DOS directory.

If an undefined password is given, the program will give you the option to create a new formula directory. **Caution:** The program uses a fixed size for the two files that are created for each directory (Appendix A) and each directory uses over 1.6 Mb of disk space.

```
*99

ALL FORMULA DIRECTORIES REQUIRE A PASSWORD -

A NEW PASSWORD WILL INITIALIZE A NEW DIRECTORY -

ENTER PASSWORD (4 char) [GSC1]: DEV2


DEV2: IS A NEW PASSWORD
DO YOU WANT TO INITIALIZE A NEW DIRECTORY? [Y/N]: Y

FORMATTING STORAGE FILES FOR FORMULAE
 10 RECORDS FORMATTED
 20 RECORDS FORMATTED
 30 RECORDS FORMATTED
 40 RECORDS FORMATTED
 50 RECORDS FORMATTED
 60 RECORDS FORMATTED
 70 RECORDS FORMATTED
 80 RECORDS FORMATTED
 90 RECORDS FORMATTED
100 RECORDS FORMATTED
```

00) CHANGE ANALYSIS DIRECTORY

Changes the working data buffer to be accessed by 11) ANALYSIS DIRECTORY , 22) OUTPUT RESULTS , 33) ENTER WT.% , 44) EDIT ANALYSES , 55) PRINT RAW DATA , 66) DELETE ANALYSES , 77) LOAD FROM ASCII FILE and 88) WRITE TO ASCII FILE.

Provision has been made for multiple directories of stored analyses where each directory has a size limit of 500 analyses and a four character password. The password of the active directory is shown in brackets in the title line of its displayed directory (11) ANALYSIS DIRECTORY).

The analysis directory password is always set to GSC1 at run-time. The example compositions used in this documentation are included in the installation copy under the password DOCU. See Appendix A for details on how to change any passworded directory into the default (GSC1) directory.

There is no command in the program that will reveal the number of analysis directories that have been created and their passwords. See Appendix A for details on how to obtain this information from the DOS directory.

If an undefined password is given, the program will give you the option to create a new analysis directory.

```
*00

ALL ANALYSIS DIRECTORIES REQUIRE A PASSWORD -

A NEW PASSWORD WILL INITIALIZE A NEW DIRECTORY -

ENTER PASSWORD (4 char) [GSC1]: JOHN


JOHN: IS A NEW PASSWORD
DO YOU WANT TO INITIALIZE A NEW DIRECTORY? [Y/N]: Y
FORMATTING STORAGE FILES FOR ANALYSES
100 RECORDS FORMATTED
200 RECORDS FORMATTED
300 RECORDS FORMATTED
400 RECORDS FORMATTED
500 RECORDS FORMATTED
```

REFERENCES

1) Deer W.A., Howie R.A. and Zussman J.; Rock Forming Minerals; 5 vols.; Longmans, Green and Co. ltd.; London (1962).

2) Pringle G.J.; EDDI: A FORTRAN Computer Program to Produce Corrected Microprobe Analyses of Minerals Using an Energy Dispersive x-ray Spectrometer; Geological Survey of Canada Open File 2127 (1989).

APPENDIX A: DOS FILES IN THE MINREP SYSTEM

```
ANDIDOCU.        4000  06/30/95 11:59
ANDIGSC1.        4000  06/30/95 11:59
SANADOCU.       75000  06/30/95 11:59
SANAGSC1.       75000  06/30/95 11:59
```

The files ANDIXXXX and SANAXXXX are matched pairs that each contain one working data buffer of 500 analyses. They are accessed in the program by means of a four character password (XXXX). On installation, (GSC1) has no data and (DOCU) has the compositions used as examples in this documentation. The program defaults to (GSC1) at run-time. Buffer (XXXX) can be made the run-time default by renaming or copying the two files to (GSC1). The DOS Copy/Rename command can also be used to backup or archive the buffers. See `00) CHANGE ANALYSIS DIRECTORY` in chapter 4 (Command descriptions).

```
FODIDOCU.        1600  06/30/95 11:59
FODIGSC1.        1600  06/30/95 11:59
SFORDOCU.     1600000  06/30/95 11:59
SFORGSC1.     1600000  06/30/95 11:59
```

The files FODIXXXX and SFORXXXX are matched pairs that each contain one set of 100 formula definitions. They are accessed in the program by means of a four character password (XXXX). On installation, (GSC1) contains a set of frequently used formulae and (DOCU) has the set used as examples in this documentation. The program defaults to (GSC1) at run-time. Set (XXXX) can be made the run-time default by renaming or copying the two files to (GSC1). The DOS Copy/Rename command can also be used to backup or archive the sets. See `99) CHANGE FORMULA DIRECTORY` in the chapter 4 (Command descriptions).

```
PRNCOD  .         640  06/30/95 11:59
```

Binary file with printer control codes.

```
ATNO    .         184  06/30/95 11:59
ATWT    .         368  06/30/95 11:59
VALE    .         184  06/30/95 11:59
```

Files with atomic numbers, atomic weights and default valences.

```
CMMT    .TXT      122  06/30/95 11:59
```

Buffer for table headers.

```
DUMP    .         3733  06/30/95 11:59
```

Buffer containing an ASCII copy of the last table to be printed. This file is constantly being overwritten. There is provision in the program to create uniquely named versions of this file.

```
MR      .EXE   328138  06/30/95 11:59
```

MINREP executable.

```
CONVTAB .EXE    45878  06/30/95 11:59
```

A utility program to convert named dump files from column format into line format or NewPet format.

```
ARROW   .WPG      206  06/30/95 11:59
MANUAL  .WPD   322855  06/30/95 11:59
```

Operators manual in WP 5.1 format

APPENDIX B: FORMULA CALCULATIONS

Example 1:

Chalcopyrite analysis where the formula is calculated as mols of each element and then scaled to an arbitrary total number of atoms.

Table 1: Chalcopyrite $CuFeS_2$ Formula basis (FNO) = 4 atoms

	wt.%	atomic weight	mols	atoms
S	35.02	32.064	1.0922	2.000
Fe	30.66	55.850	.5490	1.005
Co	0.00	58.930	.0000	.000
Ni	0.00	58.710	.0000	.000
Cu	34.54	63.540	.5436	.995
Zn	0.00	65.370	.0000	.000
Total	100.22		2.1848	4.000

mols = wt.% / at. wt.
scale factor (SF) = FNO / Σ mols = 4 / 2.1848 = 1.8308
atoms = mols x SF

Most microprobe analyses do not include a determination of oxygen and many analyses consist of determinations of cationic species only. When oxygen is a major constituent of the mineral, the structure consists of a framework that has general charge balance between the cations and negatively charged oxygen. Analyses of such minerals are frequently reported as wt.% oxides, thereby incorporating a stoichiometric amount of oxygen as an estimate of the real oxygen content.

Example 2:

Orthoclase analysis expressed as oxides. The formula is calculated as mols of each element and then scaled to the oxygen content required for charge balance.

Table 2: Orthoclase $KAlSi_3O_8$ Formula basis (FNO) = 8

	wt.%	molec. weight	mols oxide	mols oxygen	mols cation	atoms formula
SiO_2	64.84	60.09	1.0790	2.1580	1.0790	3.019
Al_2O_3	17.42	101.96	.1709	.5127	.3418	.956
Na_2O	.78	61.98	.0126	.0126	.0252	.071
CaO	0.00	56.08	.0000	.0000	.0000	.000
K_2O	15.25	94.20	.1619	.1619	.3238	.906
FeO	.98	71.85	.0136	.0136	.0136	.038
Total	99.27			2.8588		4.990

mols oxide	=	wt.% / mol.wt.
mols oxygen	=	mols oxygen associated with each cation
	=	mols oxide x oxygen subscript in oxide species
mols cation	=	mols oxide x cation subscript in oxide species
scale factor (SF)	=	FNO / Σ mols oxygen = 8 / 2.8588 = 2.7984
atoms	=	mols cation x SF

Anionic species such as OH^-, F^- and Cl^- frequently substitute for oxygen in mineral structures. There are two commonly used approaches to calculating mineral formulae under these circumstances.

The first approach is to achieve charge balance by visualizing a two for one substitution of OH^-, F^-, Cl^-, etc. for O^{-2}, and scaling on a formula basis of (FNO) oxygen equivalents. This is the usual approach when recasting x-ray spectrometer analyses where H, He and Li cannot be determined and elements from Be to Ne are frequently not determined.

The second approach is the traditional formula calculation that is used when a total analysis is available. Numerous examples of this scheme are available in Deer, Howie and Zussman (1962). In this scheme the formula is scaled on a formula basis of total anions, without regard to the value of the charge on each anionic species.

A major objective of these calculations is to test the quality of an analysis by recasting it as a mineral formula and comparing it with the stoichiometry required by the mineral structure. To this end, it is desirable to make the calculated atoms of an element in the formula to be a function of all the other element determinations. The method of scaling the formula to oxygen equivalents has a disadvantage in that the halogen analytical results do not influence the scaling factor and therefore have no influence on the formula units determined for the other elements. The method of scaling to total anions involves all the species in the formula but is of limited use in microprobe analyses when the light elements have not been determined.

Example 3:

Sodalite analysis with a univalent anion (Cl^-) in the structure. Tables 3a and 3b demonstrate that the results of the alternate schemes are numerically identical in the case where oxygen is replaced by halogens.

Table 3a: Sodalite $Na_8[Al_6Si_6O_{24}]Cl_2$ Formula basis (FNO) = 25 oxygen equivalents

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula
Na_2O	25.58	.4127	.4127	.8254	7.998
Al_2O_3	31.56	.3095	.9285	.6190	5.998
SiO_2	37.22	.6194	1.2388	.6194	6.002
Cl	7.32			(.2065)[1]	2.001
Total	101.68		2.5800		21.999
O≡Cl	(1.65)[2]				
Total	100.03				

SF = 25 / 2.58 = 9.6899

[1] mols Cl = wt.% Cl / atomic weight Cl

[2] The amount of oxygen estimated by expressing the analysis as charge balanced oxide species is too high by .2065 / 2 = .1033 mols oxygen. The correction to the total is therefore .1033 x 16 = 1.65 wt.% oxygen.

Table 3b: Sodalite $Na_8[Al_6Si_6O_{24}]Cl_2$ Formula basis (FNO) = 26(O,Cl) = total anions

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula
Na_2O	25.58	.4127	.4127	.8254	7.998
Al_2O_4	31.56	.3095	.9285	.6190	5.998
SiO_2	37.22	.6194	1.2388	.6194	6.002
Cl	7.32		(.1033)[1]	.2065	2.001
Total	101.68		2.6833		21.999
O≡Cl	1.65				
Total	100.03				

[1] In the charge balance the oxygen is overestimated by 1/2 x mols Cl. The value for 26(O,Cl) becomes: oxygen from oxide species - 1/2 x mols Cl + mols Cl

= .4127 + .9285 + 1.2388 - .10325 + .2065

= .4127 + .9285 + 1.2388 + .1033

= 2.6833

SF = 26 / 2.6833 = 9.6896

Hydrogen commonly occurs in mineral structures as the $(OH)^-$ radical or as H_2O groups. The $(OH)^-$ substitutes for oxygen in the structure and therefore is an integral part of the charge balance. Zeolitic water ($.nH_2O$ n=1,2,3...) is more loosely bonded and not directly involved in the charge balance. Some minerals contain adsorbed water which is given off on drying at 120 degrees C and reported as H_2O^-. On ignition, the $(OH)^-$ and zeolitic water are given off and reported as H_2O^+.

Example 4:

Serpentine analysis ($Mg_3[Si_2O_5](OH)_4$ Deer, Howie and Zussman (1962); vol. 3, p. 176, anal.#2) with water in the structure as $(OH)^-$. Table 4a is the formula scaled on the basis of the total anions. Table 4b reflects the fact that water and iron oxidation state cannot be determined on a microprobe and the calculation is based on oxygen equivalents. The results are not numerically identical because $(OH)^-$ is involved, unlike the previous example where the anionic substitution was by halogen only. There is a further small difference in the results introduced by the conversion of Fe_2O_3 to FeO.

Table 4a: Serpentine $Mg_3[Si_2O_5](OH)_4$ Formula basis (FNO) = 9(O,OH)

wt.%	mols oxide	mols oxygen	mols cation	atoms formula				
SiO_2	41.97	.6985	1.3970	.6985	1.942	Si	1.942	
Al_2O_3	.10	.0010	.0030	.0020	.006	Al	.006	
Fe_2O_3	.38	.0024	.0072	.0048	.013	Fe^{+3}	.013	
FeO	1.57	.0218	.0218	.0218	.061			1.961
MgO	42.50	1.0543	1.0543	1.0543	2.931	Fe^{+2}	.061	
K_2O	.08	.0008	.0008	.0016	.004	Mg	2.931	
H_2O	13.56	.7527	.7527	1.5054	4.186	K	.004	
								2.996
Total	100.16		3.2368		9.143	(OH)	4.186*	

SF = 9 / 3.2368 = 2.7805

* Hydrogen is listed with the cations as (OH) to reflect the fact that it substitutes in the structure in this form.

Table 4b: Serpentine $Mg_3[Si_2O_5](OH)_4$ Formula basis (FNO) = 7

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula			
SiO_2	41.97	.6985	1.3970	.6985	1.970	Si	1.970	
Al_2O_3	.10	.0010	.0030	.0020	.006	Al	.006	
FeO	1.91	.0266	.0266	.0266	.075			1.976
MgO	42.50	1.0543	1.0543	1.0543	2.974	Fe	.075	
K_2O	.08	.0008	.0008	.0016	.005	Mg	2.974	
						K	.005	
Total	86.56		2.4817		5.030			3.054

SF = 7 / 2.4817 = 2.8206

Example 5:

Analcime ($Na[AlSi_2O_6]\cdot H_2O$ Deer, Howie and Zussman (1962); V.4, p.343, anal.# 2) has a structure with zeolitic water. The formula can be calculated on a total anion basis if there is a reliable water determination. The formula must be calculated on an anhydrous basis when the water determination is not reliable or when there is no determination available.

Table 5a: Analcime $Na[AlSi_2O_6]\cdot H_2O$ Formula basis (FNO) = 7

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula
SiO_2	56.42	.9389	1.8778	.9389	2.039
Al_2O_3	22.21	.2178	.6534	.4356	.946
Na_2O	13.02	.2101	.2101	.4202	.913
H_2O	8.67	.4812	.4812	.9624	2.091
Total	100.32		3.2225		5.989

SF = 7 / 3.2225 = 2.1722

Table 5b: Analcime $Na[AlSi_2O_6]\cdot H_2O$ Formula basis (FNO) = 6

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula
SiO_2	56.42	.9389	1.8778	.9389	2.055
Al_2O_3	22.21	.2178	.6534	.4356	.953
Na_2O	13.02	.2101	.2101	.4202	.920
Total	91.65		2.7413		3.928

SF = 6 / 2.7413 = 2.1887

Example 6:

Smectite $(½Ca,Na)_{0.7}(Al,Mg,Fe)_4(Si,Al)_8O_{20}(OH)_4 \cdot nH_2O$ has a variable amount of non-structural water as well as an OH^- component. In this example (Deer, Howie and Zussman (1962); vol.3, p233, anal.#8) the H_2O^- value is the water lost on drying and does not enter into formula considerations. The H_2O^+ value comprises both the OH^- and the $\cdot nH_2O$, rendering it impossible to separate the $(OH)_4$ in our calculation. It is possible however to calculate the formula on a water free basis and then divide the water.

Table 6: Smectite $(½Ca,Na)_{0.7}(Al,Mg,Fe)_4(Si,Al)_8O_{20}(OH)_4 \cdot nH_2O$ Formula basis (FNO) = 22

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula			
SiO_2	45.83	.7627	1.5254	.7627	7.083	Si	7.083	
TiO_2	.46	.0058	.0116	.0058	.054	Al	.917	
Al_2O_3	22.79	.2235	.6705	.4470	4.151			8.000
Fe_2O_3	5.71	.0358	.1074	.0716	.665	Al	3.234	
FeO	.28	.0039	.0039	.0039	.036	Ti	.054	
MgO	.86	.0213	.0213	.0213	.198	Fe^{+3}	.665	
CaO	1.41	.0251	.0251	.0251	.233	Fe^{+2}	.036	
Na_2O	.16	.0026	.0026	.0052	.048	Mg	.198	
K_2O	.09	.0010	.0010	.0020	.019			4.187
H_2O^+	9.79					Ca	.233	
H_2O^-	12.55					Na	.048	
						K	.019	
Total	99.93		2.3688					.300
						OH	(4.000)[1]	
						H_2O	(3.046)[2]	

SF = 22 / 2.3688 = 9.2874

[1] assumed

[2] to estimate n = formula units $n \cdot H_2O$,

units OH / SF = mols OH = 4.000 / 9.2874 = .4307

wt.% H_2O associated with OH = .4307 / 2 x mol.wt. H_2O
= .2154 x 18.016
= 3.88

wt.% as $n \cdot H_2O$ = wt.% H_2O^+ - 3.88 = 5.91 = .3280 mols

n = .328 x SF = 3.046

Example 7:

Phlogopite $K_2(Mg,Fe^{+2})_6[Si_6Al_2O_{20}](OH,F)_4$ with anion substitutions of (F^-) and (OH^-) both of which are not usually available for inclusion in a microbeam x-ray analysis. The example (Deer, Howie and Zussman (1962); vol.3, p.46, anal.#2) is calculated first as presented and then on an anhydrous basis.

Table 7a: Phlogopite $K_2(Mg,Fe^{+2})_6[Si_6Al_2O_{20}](OH,F)_4$ FNO = 24(O,OH,F)

	wt.%	mols oxide	mols oxygen	mols cations	atoms formula			
SiO_2	41.18	.6853	1.3706	.6853	5.826	Si	5.826	
Al_2O_3	12.52	.1228	.3684	.2456	2.088	Al	2.088	
TiO_2	.99	.0124	.0248	.0124	.105	Ti	.086	
FeO	.30	.0042	.0042	.0042	.036			8.000
MnO	.04	.0006	.0006	.0006	.005	Ti	.019	
MgO	27.32	.6777	.6777	.6777	5.761	Fe	.036	
Na_2O	.88	.0142	.0142	.0248	.241	Mn	.005	
K_2O	11.93	.1266	.1266	.2532	2.152	Mg	5.761	
F	6.74		(.1774)	.3547	3.015			5.821
H_2O^+	1.06	.0588	.0588	.1176	1.000	Na	.241	
						K	2.152	
Total	102.96		2.8233					2.393
						F	3.015	
O≡F		2.84					OH	1.000
								4.015
Total	100.12							

SF = 24 / 2.8233 = 8.5007

Table 7b: Phlogopite $K_2(Mg,Fe^{+2})_6[Si_6Al_2O_{20}](OH,F)_4$ FNO = 22 oxygen equivalents

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula			
SiO_2	41.18	.6853	1.3706	.6853	5.828	Si	5.828	
Al_2O_3	12.52	.1228	.3684	.2456	2.089	Al	2.089	
TiO_2	.99	.0124	.0248	.0124	.105	Ti	.083	
FeO	.30	.0042	.0042	.0042	.036			8.000
MnO	.04	.0006	.0006	.0006	.005	Ti	.022	
MgO	27.32	.6777	.6777	.6777	5.763	Fe	.036	
Na_2O	.88	.0142	.0142	.0284	.242	Mn	.005	
K_2O	11.93	.1266	.1266	.2532	2.153	Mg	5.763	
								5.826
Total	95.16		2.5871			Na	.242	
						K	2.153	
								2.395

SF = 22 / 2.5871 = 8.5037

Example 8:

Tourmaline $Na(Mg,Fe,Mn,Al)_3Al_6[Si_6O_{18}](BO_3)_3(OH,F)_4$ contains Boron which is not routinely analyzed with x-ray spectrometers. Also included are F^- and OH^- which are frequently not analyzed. The example (Deer, Howie and Zussman (1962); vol.1, p.304, anal.#1) is first calculated with the determined values for Boron and water. Fluorine is absent in this particular example. Compare this with the result in Table 8b which is calculated as if the light element results were not available.

Table 8a: Tourmaline $Na(Mg,Fe,Mn,Al)_3Al_6[Si_6O_{18}](BO_3)_3(OH,F)_4$ FNO = 31(O,OH,F)

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula			
SiO_2	35.96	.5984	1.1986	.5984	5.758	Si	5.758	
B_2O_3	10.73	.1541	.4623	.3082	2.966	B	2.966	
Al_2O_3	30.85	.3026	.9078	.6052	5.824	Al	5.824	
TiO_2	.14	.0018	.0036	.0018	.017			14.548
MgO	13.67	.3391	.3391	.3391	3.263	Al	.000	
FeO	.76	.0106	.0106	.0106	.102	Mg	3.263	
Na_2O	1.63	.0263	.0263	.0526	.506	Ti	.017	
CaO	2.41	.0430	.0430	.0430	.414	Fe	.102	
K_2O	.09	.0010	.0010	.0020	.019	Na	.506	
H_2O^+	4.16	.2309	.2309	.4618	4.444	Ca	.414	
						K	.019	
Total	100.40		3.2214					4.321
						OH	4.444	

SF = 31 / 3.2214 = 9.6231

Removing B and OH from consideration we calculate on the basis of FNO = 49 oxygen equivalents. Since boron is given as B_2O_3 in the analysis there are 1.5 oxygens associated with each atom of boron. In this case -

FNO = (31 - 4(OH,F) - 3 x 1.5 + 2) x 2
= (31 - 2 - 4.5) x 2
= 24.5 x 2
= 49

Table 8b: Tourmaline $Na(Mg,Fe,Mn,Al)_3Al_6[Si_6O_{18}](BO_3)_3(OH,F)_4$ FNO = 49 oxygen equivalents

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula			
SiO_2	35.96	.5984	1.1968	.5984	11.598	Si	5.799	
Al_2O_3	30.85	.3026	.9078	.6052	11.730	Al	5.865	
TiO_2	.14	.0018	.0036	.0018	.035			11.664
MgO	13.67	.3391	.3391	.3391	6.572	Al	.000	
FeO	.76	.0106	.0106	.0106	.205	Mg	3.286	
Na_2O	1.63	.0263	.0263	.0520	1.008	Ti	.018	
CaO	2.41	.0430	.0430	.0430	.833	Fe	.103	
K_2O	.09	.0010	.0010	.0020	.039	Na	.504	
						Ca	.417	
Total	85.51		2.5282			K	.020	
								4.348

SF = 49 / 2.5282 = 19.3814

Example 9:

End member molecules calculated using Labradorite as an example.

Table 9: Labradorite $(Na,Ca)(Al_{1-2}Si_{3-2})O_8$ FNO = 32

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula			
SiO_2	51.90	.8637	1.7274	.8637	9.450	Si	9.450	
Al_2O_3	30.45	.2986	.8958	.5972	6.534	Al	6.534	
Na_2O	3.86	.0623	.0623	.1246	1.363			15.984
CaO	13.04	.2325	.2325	.2325	2.544	Na	1.363	
K_2O	.18	.0019	.0019	.0038	.042	Ca	2.544	
FeO	.35	.0049	.0049	.0049	.054	K	.042	
								3.949
Total	99.78		2.9248					

SF = 32 / 2.9248 = 10.9409

For three end members -

	formula	cation associated with end member
Albite	$NaAlSi_3O_8$	Na
Anorthite	$CaAl_2Si_2O_8$	Ca
Orthoclase	$KAlSi_3O_8$	K

	(1) mol.wt.	(2) mols cation	(3) mols	(4) wt.%	(5) mol.%
Albite	262.240	.1246	.1246	32.68	34.52
Anorthite	278.220	.2325	.2325	64.69	64.42
Orthoclase	278.352	.0038	.0038	1.06	1.05
Total			.3609	98.43	

mols end member (3) = mols cation (2) / cation subscript in end member formula

wt.% end member (4) = mols end member (3) x end member molecular weight (1)

mol.% end member (5) = (mols end member (3) / Σ mols end members) x 100.

Example 10:

Garnet end members. The Fe_2O_3 and FeO are calculated from total Fe as 30.29 wt.% FeO, as in Appendix C.

Table 10: Garnet $(Mg,Fe^{+2},Mn,Ca)_3(Cr,Fe^{+3},Ti,Al)_2(Ti,Al,Si)_3O_{12}$ FNO = 24

	wt.%	mols oxide	mols oxygen	mols cation	atoms formula			
SiO_2	37.76	.6284	1.2568	.6284	5.972	Si	5.972	
Al_2O_3	20.75	.2035	.6105	.4070	3.868	Al	.028	
TiO_2	.14	.0017	.0034	.0017	.016	Ti	.000	
Fe_2O_3	1.28	.0080	.0240	.0160	.152			6.000
Cr_2O_3	.07	.0005	.0015	.0010	.010	Al	3.840	
MgO	2.89	.0717	.0717	.0717	.681	Ti	.016	
FeO	29.14	.4056	.4056	.4056	3.855	Fe^{+3}	.152	
MnO	1.22	.0172	.0172	.0172	.163	Cr	.010	
CaO	7.52	.1341	.1341	.1341	1.275			4.018
K_2O	.04	.0004	.0004	.0008	.008	Mg	.681	
						Fe^{+2}	3.855	
Total	100.81				16.000[1]	Mn	.163	
						Ca	1.275	
						K	.008	
								5.982

SF = 24 / 2.5252 = 9.5042

[1] Fixed by the calculation of Fe^{+3} and Fe^{+2}

For seven end members -

	formula	cation associated with end member
Almandine	$Fe^{+}{}_{3}{}^{2}Al_2Si_3O_{12}$	Fe^{+2}
Andradite	$Ca_3Fe^{+}{}_{2}{}^{3}Si_3O_{12}$	Fe^{+3}
Schorlomite	$Ca_3Ti_2Si_3O_{12}$	Ti
Grossular	$Ca_3Al_2Si_3O_{12}$	Ca
Pyrope	$Mg_3Al_2Si_3O_{12}$	Mg
Spessartine	$Mn_3Al_2Si_3O_{12}$	Mn
Uvarovite	$Ca_3Cr_2Si_3O_{12}$	Cr

		(1) mol.wt.	(2) mols cation	(3) mols	(4) wt.%	(5) mol%
Alman	Fe^{+2}	497.78	.4056	.1353	67.35	64.52
Andra	Fe^{+3}	508.21	.0160	.0080	4.07	3.82
Schlm	Ti	547.83	.0017	.0009	.49	.43
Gross	Ca	450.47	(.1061)[1]	.0354	15.95	16.89
Pyrop	Mg	403.16	.0717	.0239	9.64	11.35
Spess	Mn	495.05	.0172	.0057	2.82	2.72
Uvaro	Cr	500.41	.0010	.0005	.25	.24
Total				.2097	100.57	

[1] $Ca - 1.5Cr - 1.5Ti - 1.5Fe^{+3} = .1061$

mols end member (3) = mols cation (2) / cation subscript in end member formula

wt.% end member (4) = mols end member (3) x mol. wt. end member (1)

mol% end member (5) = (mols end member (3) / Σ mols end members) x 100.

Example 11:

Chromite end members.

Table 11: Chromite $(Fe,Mg,Mn)(Fe,Cr,Al,Ti)_2O_4$ FNO = 32

	wt.%	mols oxide	mols oxygen	mols cations	atoms formula			
TiO_2	.93	.0117	.0234	.0117	.187	Ti	.187	
Al_2O_3	14.43	.1415	.4245	.2830	4.528	Al	4.528	
Cr_2O_3	36.61	.2409	.7227	.4818	7.708	Cr	7.708	
Fe_2O_3	16.92	.1059	.3177	.2118	3.389	Fe^{+3}	3.389	
FeO	23.19	.3228	.3228	.3228	5.165			15.812
MgO	7.47	.1853	.1853	.1853	2.965	Fe^{+2}	5.165	
MnO	.26	.0037	.0037	.0037	.059	Mg	2.965	
						Mn	.059	
Total	99.81		2.0001					8.189

SF = 32 / 2.0001 = 15.9992

For nine end members -

		mol.wt.	mols[1]	wt.%	mol%
Magnesiochromite	$MgCr_2O_4$	192.31	.0921	17.71	18.42
Chromite	$Fe^{+2}Cr_2O_4$	223.85	.1488	33.31	29.76
Spinel	$MgAl_2O_4$	142.27	.0537	7.64	10.74
Hercynite	$Fe^{+2}Al_2O_4$	173.81	.0867	15.07	17.34
Galaxite	$MnAl_2O_4$	172.90	.0011	.19	.22
Magnesioferrite	$MgFe^{+}{}_2{}^3O_4$	200.01	.0402	8.04	8.04
Magnetite	$Fe^{+2}Fe^{+}{}_2{}^3O_4$	231.55	.0649	15.03	12.98
Jacobsite	$MnFe^{+}{}_2{}^3O_4$	230.64	.0008	.18	.16
Ulvospinel	$Fe^{+}{}_2{}^2TiO_4$	223.60	.0117	2.62	2.34
Total			.5000	99.79	

[1] in mols -

$MgCr_2O_4 + Fe^{+2}Cr_2O_4 = Cr / 2$
$MgAl_2O_4 + Fe^{+2}Al_2O_4 + MnAl_2O_4 = Al / 2$
$MgFe^{+}{}_2{}^3O_4 + Fe^{+2}Fe^{+}{}_2{}^3O_4 + MnFe^{+}{}_2{}^3O_4 = Fe^{+3} / 2$

$MgCr_2O_4 = (Cr / 2) \times Mg / (Mg + Fe^{+2} - 2Ti)$
$Fe^{+2}Cr_2O_4 = (Cr / 2) \times (Fe^{+2} - 2Ti) / (Mg + Fe^{+2} - 2Ti)$
$MgAl_2O_4 = (Al / 2) \times Mg / (Mg + Fe^{+2} - 2Ti + Mn)$
$Fe^{+2}Al_2O_4 = (Al / 2) \times (Fe^{+2} - 2Ti) / (Mg + Fe^{+2} - 2Ti + Mn)$
$MnAl_2O_4 = (Al / 2) \times Mn / (Mg + Fe^{+2} - 2Ti + Mn)$
$MgFe^{+}{}_2{}^3O_4 = (Fe^{+}3 / 2) \times Mg / (Mg + Fe^{+2} - 2Ti + Mn)$
$Fe^{+2}Fe^{+}{}_2{}^3O_4 = (Fe^{+3} / 2) \times (Fe^{+2} - 2Ti) / (Mg + Fe^{+2} - 2Ti + Mn)$
$MnFe^{+}{}_2{}^3O_4 = (Fe^{+3} / 2) \times Mn / (Mg + Fe^{+2} - 2Ti + Mn$
$Fe^{+}{}_2{}^2TiO_4 = Ti$

APPENDIX C: CALCULATION OF FE^{+2},FE^{+3} BY STOICHIOMETRY

It is often necessary to arbitrarily express Fe^{total} as either FeO or Fe_2O_3 since the oxidation state is not determined in microbeam x-ray analysis. However, if enough is known about the crystal chemistry of the material, it is sometimes possible to estimate the division between valences by assuming ideal formula contents in the various substitution sites.

Table 1 is an amphibole analysis where Fe^{+2} and Fe^{+3} have been analytically determined. The aluminium is arbitrarily divided between the first and second sites by filling the first site and then putting the balance in the second site.

Table 1: Amphibole (Deer, Howie and Zussman; vol.2, p.275, #6)

	wt.% oxide	mols oxide	mols oxygen	mols cation		atoms formula	
SiO_2	52.78	.8783	1.7566	.8783	Si	7.389	
TiO_2	.43	.0054	.0108	.0054	Ti	.045	
Al_2O_3	5.77	.0566	.1698	.1132	Al	.566	
Fe_2O_3	2.45	.0153	.0459	.0306			8.000
FeO	6.61	.0920	.0920	.0920	Al^{+3}	.386	
MnO	.17	.0024	.0024	.0024	Fe^{+3}	.257	
MgO	17.43	.4324	.4324	.4324	Fe^{+2}	.774	
CaO	11.90	.2122	.2122	.2122	Mn	.020	
Na_2O	.68	.0110	.0110	.0220	Mg	3.638	
K_2O	.07	.0007	.0007	.0014			5.075
					Ca	1.785	
Total	98.29		2.7338		Na	.185	
					K	.012	
							1.982

The division of Al between two sites does not imply that Al is in two oxidation states.

The ideal formula is -

$$(Na,K,Ca)_2(Mg,Fe^{+2},Fe^{+3},Al)_5(Si,Al)_8O_{22}(OH,F)_2$$

giving -

$$SF = FNO / \Sigma O$$

$$= 23 / 2.7338 = 8.4132$$

Table 2 is the same analysis with total Fe as FeO as if it were obtained on a microbeam instrument with an x-ray spectrometer.

Table 2: Amphibole from Table 1 with Fe^{total} = FeO

	wt.% oxide	mols oxide	mols oxygen	mols cation		atoms formula	
SiO_2	52.78	.8783	1.7566	.8783	Si	7.431	
TiO_2	.43	.0054	.0108	.0054	Ti	.046	
Al_2O_3	5.77	.0566	.1698	.1132	Al	.523	
FeO	8.81	.1226	.1226	.1226			8.000
MnO	.17	.0024	.0024	.0024	Al	.435	
MgO	17.43	.4324	.4324	.4324	Fe	1.037	
CaO	11.90	.2122	.2122	.2122	Mn	.020	
Na_2O	.68	.0110	.0110	.0220	Mg	3.658	
K_2O	.07	.0007	.0007	.0014			5.150
	-----		-----		Ca	1.795	
Total	98.04		2.7185		Na	.186	
					K	.012	
							1.993

SF = FNO / ΣO = 23 / 2.7185 = 8.4605

It is possible to calculate values for Fe^{+2} and Fe^{+3} that give the closest fit to stoichiometry by assuming an ideal total in one or more formula sites. The sites used to base the calculation are called the determining sites in the development below.

When total iron is expressed as Fe^{+2} (TF), stoichiometry is achieved by converting some Fe^{+2} to Fe^{+3} (FC). In cases where TF is as Fe^{+3}, then FC becomes Fe^{+2}.

Define an index variable to have the values -

S2 = (Valence of FC) x 2 - 5

= -1 when FC is +2

= +1 when FC is +3

There are four possible combinations of placement of TF and FC in the determining sites. these may be expressed by index variables as -

S3 = -1	when TF is in the determining sites
S3 = +1	when TF is not in the determining sites
S4 = -1	when FC is in the determining sites
S4 = +1	when FC is not in the determining sites

If S1 = S3 + S4

Then	S1 = 0	when both TF and FC are in the sites
	S1 = 0	when both TF and FC are not in the sites
	S1 = -2	when TF is in the sites and FC is not in the sites
	S1 = +2	when TF is not in the sites and FC is in the sites

The form and values of the index variables S1 and S2 are chosen to provide a convenient link between the conditional tests in the program code and the calculation expressions developed below.

Define -

M_1	=	Σ mols cation in the determining sites before iron is divided
M_2	=	Σ mols cation in the determining sites after iron is divided
S_1	=	Σ of the atoms for the determining sites in the formula, before iron is divided
S_2	=	Σ of the atoms for the determining sites in the formula (theoretical)
FNO	=	number of oxygens used as the normalization basis for the formula
Q_1	=	Σ mols oxygen in the analysis before iron is divided
SF	=	scaling factor before iron is divided
Q_2	=	Σ mols oxygen in the analysis after iron is divided
MF^{+2}	=	mols Fe^{+2} after iron is divided
MF^{+3}	=	mols Fe^{+3} after iron is divided

If TF is as Fe^{+2} then -

$$FC = MF^{+3}$$

and $$Q_2 = Q_1 - MF^{+2} - MF^{+3} + MF^{+2} + 1.5 \times MF^{+3}$$

$$Q_2 = Q_1 + MF^{+3} / 2 \quad (1)$$

If TF is as Fe^{+3} then -

$$FC = MF^{+2}$$

and $$Q_2 = Q_1 - 1.5 \times MF^{+2} - 1.5 \times MF^{+3} + MF^{+2} + MF^{+3}$$

$$Q_2 = Q_1 - MF^{+2} / 2 \quad (2)$$

(1) and (2) may be combined if expressed in terms of S2 and FC -

$$Q_2 = Q_1 + \frac{S2 \times FC}{2} \qquad (3)$$

also -

$$M_2 = M_1 + \frac{S1 \times FC}{2}$$

The difference in mols cation in the determining sites before and after the division of iron can be expressed as -

$$M_1 - M_2 = (S_1 \times Q_1 / FNO) - (S_2 \times Q_2 / FNO)$$

$$FNO \times (M_1 - M_1 - (S1 \times FC / 2)) = S_1 \times Q_1 - S_2 \times (Q_1 + (S2 \times FC / 2))$$

$$- (FNO \times S1 \times FC) = 2 \times S_1 \times Q_1 - 2 \times S_2 \times Q_1 - S2 \times S_2 \times FC$$

$$FC \times (S2 \times S_2 - FNO \times S1) = 2 \times Q_1 \times (S_1 - S_2)$$

$$FC = \frac{2 \times Q_1 \times (S1 - S_2)}{S2 \times S_2 - FNO \times S_1} \qquad (4)$$

Recast in terms of SF this becomes -

$$FC = \frac{2 \times FNO \times (S_1 - S_2)}{SF \times (S2 \times S_2 - S1 \times FNO)}$$

which is the form of (4) used in MINREP.

In the example given in Table 2 we have -

$$S1 = 0 \qquad S2 = +1$$

$$\text{mols } Fe^{+3} = FC = \frac{2 \times 23 \times (13.15 - 13.00)}{8.4605 \times (1 \times 13.00 - 0 \times 23)}$$

$$= .0627$$

$$\text{mols } Fe^{+2} = .1226 - .0627 = .0599$$

which are the values presented in Table 3.

Table 3: Calculated Fe^{+3}
Amphibole (Deer, Howie and Zussman; vol.2, p.275, #6)

	wt.% oxide	mols oxide	mols oxygen	mols cation		atoms formula	
SiO_2	52.78	.8783	1.7566	.8783	Si	7.346	
TiO_2	.43	.0054	.0108	.0054	Ti	.045	
Al_2O_3	5.77	.0566	.1698	.1132	Al	.609	
Fe_2O_3	5.01	.0314	.0942	.0628			8.000
FeO	4.30	.0599	.0599	.0599	Al	.338	
MnO	.17	.0024	.0024	.0024	FC	.525	
MgO	17.43	.4324	.4324	.4324	FE	.501	
CaO	11.90	.2122	.2122	.2122	Mn	.020	
Na_2O	.68	.0110	.0110	.0220	Mg	3.616	
K_2O	.07	.0007	.0007	.0014			5.000
					Ca	1.775	
Total	98.54		2.7500		Na	.184	
					K	.012	
							1.971

APPENDIX D: DATA FILE FORMAT

The characteristics of the data files read into MINREP via 77) LOAD FROM ASCII FILE or written to disk via 88) WRITE TO ASCII FILE are -

1) ASCII (DOS text) format.
2) One record per analysis.
3) Comma delimiters in characters 12,21,30,39,.....
4) An eight character label in characters 3 to 10 with quotes in characters 2 and 11.
5) Data as decimal numbers, the decimal as ch# 17,26,35,.... etc. and a data field of eight characters.
6) A maximum of 20 analyzed elements for non-oxide format and a maximum of 19 analyzed elements for oxide format.
7) The keyword "SAMPLE " in the label field identifies the record as a format record giving the chemical species labels for the data fields in succeeding data records. There may be several blocks of data in the same file, if each is preceded by a label record. Blocks of data in the same file do not need to have the same structure. The first record in any data file must be a format record and the program will read records in this format until another SAMPLE record is encountered. If the first record is not a format record then the program will skip data until a format record is reached.
8) If character 15 in a format record is blank then the program reads the data in non-oxide format, otherwise it uses oxide format.
9) The program counts the number of chemical species in the coming block of data by looking for the keywords " TOTAL " or " TOTAL," in the format record. 77) LOAD ASCII does not read the analysis totals. 88) WRITE ASCII includes a total in the output.
10) 88) WRITE ASCII optionally includes a terminating comma on each record immediately after the last data field.

This is a format that DBASE will accept. Other database and spreadsheet programs should be able to accommodate it with little if any modification. In some cases these programs import data more cleanly if the final comma in each record is omitted.

SAMPLE	CU	AS	SE	SB	S	ZN	FE	CD	PB	MN	NI	CO	TOTAL
"JUNK0001"	0.000	0.055	0.000	0.000	51.482	0.042	48.378	0.000	0.000	0.000	0.038	0.029	100.024
"JUNK "	000.000	000.055	000.000	000.000	051.482	000.042	048.378	000.000	000.000	000.000	000.038	000.029	100.024
"A101 "	000.084	000.029	000.079	000.000	032.633	051.842	015.580	000.092	000.000	000.064	000.019	000.010	100.422
"A102 "	000.448	000.000	000.043	000.018	032.734	051.065	015.571	000.076	000.000	000.064	000.019	000.011	100.049
"A103 "	000.162	000.068	000.000	000.016	032.166	052.466	014.616	000.123	000.000	000.077	000.000	000.029	99.723

SAMPLE	NA2O	K2O	FEO	MGO	SIO2	CAO	MNO	TIO2	CR2O3	AL2O3	NIO	TOTAL
"TF GTR "	.001	.019	32.888	2.353	36.259	3.637	2.765	.060	.091	19.901	.052	98.025
"TF GTC "	.000	.006	32.042	3.223	38.251	3.947	2.817	.060	.056	20.811	.037	101.251
"TR GTR "	.000	.411	30.380	2.311	32.828	4.020	2.783	.138	.069	18.145	.080	91.166
"TF GTM "	.170	.112	32.801	2.680	38.557	3.583	2.947	.007	.134	21.756	.057	102.804
"TF GTC "	.000	.000	32.449	2.855	37.284	3.634	2.646	.003	.009	20.583	.000	99.463
"TF GTR "	.000	.023	32.807	2.575	37.042	4.318	2.846	.072	.110	20.288	.107	100.187
"TF GTM "	.000	.023	32.767	3.323	39.027	3.536	2.929	.015	.066	21.945	.000	103.630
"TF GTC "	.748	.814	29.199	2.550	36.157	3.588	2.724	.088	.124	18.722	.150	94.865

SAMPLE	NA2O	K2O	MGO	FE2O3	F	SIO2	MNO	CL	BAO	CAO	AL2O3	CR2O3	NIO	TIO2	TOTAL
"BI-7C "	.044	9.587	9.392	25.356	.203	36.189	.230	.007	.269	.022	14.869	.121	.010	2.651	98.951
"HB-7R "	.927	.871	8.606	22.697	.000	44.405	.461	.059	.083	11.792	8.737	.054	.045	.744	99.483
"HB-7C "	.984	.812	9.024	22.581	.000	45.154	.487	.022	.039	11.752	7.840	.060	.000	1.386	100.141
"HB-7R "	.886	.923	8.445	22.528	.000	44.033	.524	.040	.108	11.850	8.733	.000	.099	.871	99.040