DEPARTMENT OF THE INTERIOR

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SAVEWARE I: A DOZEN PROGRAMS DESIGNED TO READ DATASAVE FILES, PERFORM VARIOUS PETROLOGIC CALCULATIONS, AND PRODUCE PRINTED AND GRAPHICAL DATA ANALYSIS

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CONTENTS

ABSTRACT

SAVEWARE is a group of 12 programs that run on IBM and IBM-compatible microcomputers. The programs were written in QuickBASIC and have been combined with input/output routines from DATASAVE. The programs (except ASCI2DSV) access data from DATASAVE format data files and perform various petrologic operations. Program names and functions are listed below:

ASCI2DSV: converts ASCII files to DATASAVE format data files
DSVECORR: computes correlation coefficients
DSVEEDIL: plots enrichment/depletion profiles
DSVEFELD: conducts feldspar geothermometric calculations
DSVEGARN: computes garnet end member proportions
DSVEMICA: computes structural formulae for micas
DSVEMINF: computes generic mineral structural formulae
DSVEREPL: plots chondrite normalized rare earth element diagrams
DSVERGRS: computes and plots linear regressions
DSVESPDR: plots extended trace element patterns
DSVEWALK: computes and plots ternary proportions in the experimental basalt system
DSVFEWAT: partitions total iron between FeO and Fe_2O_3 before storing revised major oxide data normalized to 100 percent, anhydrous

Output, both numeric and graphical, can be directed to a printer. Some of the programs allow computed or reprocessed data to be written as new DATASAVE format data files.

INTRODUCTION

The group of twelve programs described here were developed to facilitate petrologic and mineralogic calculations and graphical output for data stored in DATASAVE (Quick, 1988) format data files. These programs offer specific application extensions to the capabilities inherent in DATASAVE and are designed to read and process DATASAVE format data files without the need for file conversion. This environment was chosen for SAVEWARE because a number of U.S. Geological Survey geologists use DATASAVE software routinely.

The DATASAVE (Quick, 1988) software/database system is characterized by an open architecture. Specifically, the DATASAVE SPLICE routine allows user-created subroutines written in BASIC to be merged with the DATASAVE software that controls all data input/output functions. All of the SAVEWARE programs are "SPLICED" QuickBASIC subroutines; they can read (and where appropriate, write) DATASAVE format data files.

Familiarity with DATASAVE software is not essential though a working knowledge of those programs is helpful in running SAVEWARE programs. An understanding of the DATASAVE "codes" concept (Quick, 1988) is essential in running SAVEWARE programs. The user is referred to page 2-5 of in the DATASAVE documentation (Quick, 1988)

where standard operating conventions that are equally applicable to SAVEWARE operation are presented.

The software was developed and runs on IBM PC, XT, AT, or compatible microcomputers with at least 384 Kb (kilobytes) RAM (random access memory) and at least one disk drive. An enhanced-graphic adapter (EGA) and compatible monitor are required to run DSVEREPL, DSVESPDR, AND DSVEEDIL although DSVCREPL and DSVCSPDR (color-graphics adapter (CGA) compatible versions of the first two programs) can be implemented on machines equipped with CGA adapters and compatible monitors. DSVEWALK can be implemented only on machines capable of CGA display. DSVERGRS runs on CGA and EGA systems, as specified by the user. Graphical output from these programs can be output via Print Screen to most types of printers. RAM-resident screen printing routines such as GRAPHICS.COM (a component of IBM- and MS-DOS packages) and EGAEPSON.COM (a piece of share ware that can be downloaded from some electronic bulletin boards) must be installed in order to output CGA and EGA, respectively, screen graphic images to the printer. All of the programs run under IBM- or MS-DOS 2.0 or higher and require the QuickBASIC run-time module BRUN30.EXE, which is provided.

INSTALLATION

Two disks accompany this manual. Disk 1 contains 14 files that constitute the executable versions of SAVEWARE programs:

ASCI2DSV.EXE
DSVCREPL.EXE
DSVCSPDR.EXE
DSVECORR.EXE
DSVEEDIL.EXE
DSVEFELD.EXE
DSVEGARN.EXE
DSVEMICA.EXE
DSVEMINF.EXE
DSVEREPL.EXE
DSVERGRS.EXE
DSVESPDR.EXE
DSVEWALK.EXE
DSVFEWAT.EXE

Disk 2 contains 15 files. The first two files are necessary to run SAVEWARE programs. BRUN30.EXE is the QuickBASIC runtime module; it contains a number of routines that are called by compiled versions of SAVEWARE programs. RBVSR.SUB is a subroutine file to be used by DSVERGRS.EXE. SAVECODE is a code file (Quick, 1988) that contains the codes necessary to access data contained in the remaining files (*.DAT) on the disk. Filenames for these data files, which can be used to test or preview the operation of the associated programs, are indexed to the appropriate SAVEWARE programs:

BRUN30.EXE
SAVECODE
ASCI.DAT
REPL.DAT
SPDR.DAT
CORR.DAT
EDIL.DAT
FELD.DAT
GARN.DAT
MICA.DAT
MINF.DAT
RGRS.DAT
WALK.DAT
FEWAT.DAT
RBVSR.SUB

SAVEWARE programs are not copy protected and may be transferred to new disk using the DOS COPY command. Original disks should be copied to working disks and then placed in a safe place. Disk 1 is formatted under DOS 3.3. If SAVEWARE programs are run under DOS 3.0 or higher, it is essential that the contents of disk 1 be copied onto a disk formatted with DOS 3.0 or higher.

Two floppy drive system:

To create a bootable program disk:

1) Place a blank disk in drive B
2) Place DOS disk in drive A
3) Type FORMAT B:/S
4) Place disk 2 in drive A
5) Type COPY A:*.* B:
6) Place disk 1 in drive A
7) Type COPY a:filename.exe B:
   where "filename" is the name of the program(s) you wish to run

The resulting bootable disk now contains SAVEWARE programs. In order to run any of these programs place this disk in drive A and a disk containing your DATASAVE disk in drive B.

Hard drive system:

Create a SAVEWARE subdirectory:

1) Type MD SAVEWARE
2) Place disk 1 in drive A
3) Type CD \SAVEWARE
4) Type COPY A:*.*
5) Place disk 2 in drive A
6) Type copy A:*.*

The resulting directory, which is created as a subdirectory of the current drive and directory, now contains SAVEWARE programs and files necessary to run any of the programs. DATASAVE data files can be copied into this same subdirectory, into different subdirectories, or can be accessed from floppy disk drives.

GENERAL COMMENTS CONCERNING EXECUTION OF SAVEWARE PROGRAMS

SAVEWARE programs prompt for a drive designation (A or B) during the input file specification procedure. If data is to be read from a hard disk subdirectory, that subdirectory must be set as the default in that drive (or drive partition). Thus input data can be read from (and written to) subdirectories on drive D, E, F, etc.

The initial steps in operating all of the SAVEWARE programs, except ASCI2DSV, are similar (variants are described in appropriate Program Operation sections) and are described here to avoid redundancy. The initial menu and some of the features of DSVERGRS, which are slightly different from those of other SAVEWARE programs, are also described in the appropriate section below. To run any of the SAVEWARE programs, change to the drive or working directory that contains the programs, type the program filename, and hit the Enter key.

After a particular SAVEWARE program (e.g. DSVEREPL) has been loaded, and following display of any introductory messages associated with the particular program, an options menu is displayed:

```
PROGRAM: DSVEREPL
********** MENU **********
     S   Sample Code File
     R   Recall Data File
   Esc   Exit Program
**********************************
 Current Sample Code File: CODES
```

Hitting the Esc key causes operations to return to DOS. If the code file displayed beneath the menu is not appropriate to the data to be analyzed, select option S from the menu to begin identification of the proper code file. Input name of code file (use the code file named SAVECODE to process test data, supplied on disk 2, using any of the SAVEWARE programs) and drive designation at the appropriate prompts:

```
Sample Code File?                Drive (A or B)?
```

Program execution begins when option R is selected. Input the name and drive designation of the file to be retrieved at the prompts:

```
Data file name?                  Drive (A or B)?
                Current data file:
```

Typing DIR at the Data file name prompt and a drive designation at the drive prompt causes a directory listing of the specified drive to be displayed on the monitor (Quick, 1988). The second and all succeeding loops through SAVEWARE programs include default file name and drive designations identical to the previously identified file and drive. Defaults are specified by the highlighted "Current Data File:" message displayed below the file name and drive prompts; the defaults are selected by hitting the Enter key in

response to the filename and drive prompts. A summary of the selected file's contents is displayed:

```
There are 3 samples in the file.
 Sample code      # of samples
     INA              3
 Use this file (Y/N)?
```

Answer yes (Y) to confirm the input file designation, or no (N) to return to file and drive designation prompts. If all samples in the file are to be processed, answer yes (Y) to the prompt:

```
Run all the data (Y/N)
```

Answer no (N) to enable the SCROLLER routine (Quick, 1988), which enables selection of individual samples from the specified file. SCROLLER is operated using the key functions indicated on the bottom line of the display and is described by Quick (1988; p. 4-6). After exiting the SCROLLER, a message:

```
You are batch processing XXX analyses,
```

displays the number of samples (XXX) chosen for analysis and prompts with:

```
Hit any key to continue
```

A sequential series of messages:

```
Processing analysis number XXXXXXXXXXX
```

where XXXXXXXXXXX are the sample numbers of the entries chosen for analysis, are displayed; this message indicates data retrieval, assignment of file values to the appropriate data identifiers and transmission of data to the subroutine that will conduct data processing.

ACKNOWLEDGMENTS

IBM and IBM-DOS are trademarks of International Business Machines Corporation. MS-DOS is a trademark of Microsoft Incorporated. The QuickBASIC BRUN30.EXE runtime module is the copywrited property of Microsoft Incorporated; it may be distributed with copies of SAVEWARE as long as its name and contents are not modified. This manual and SAVEWARE programs are in the public domain. Source code can be obtained on request from E.A. du Bray, USGS MS 905; Box 25046, DFC; Denver, CO 80225.

SAVEWARE programs were developed during the last five years with the input of numerous people. The authors thank their colleagues for their willingness to have their public domain subroutines SPLICED. Specific acknowledgments are given in the descriptive sections below. This manual was improved by the review of Carl Thornber.

ASCI2DSV

Description

ASCI2DSV is a program that converts ASCII files to files that can be accessed and read by any of the DATASAVE and SAVEWARE programs. Test data for this program are in the file ASCI.DAT. Both David A. Dellinger (University of California at Santa Barbara) and Carol N. Gerlitz (USGS) provided essential input in writing this program.

The program reads files whose first line indicates the number of samples in the ASCII file and the number of observations (oxides or elements) per sample; numerical values for these two pieces of information must be separated by one or more spaces. The second and all succeeding, even-numbered lines contain a sample number up to twelve characters long. The third, and all succeeding odd-numbered lines contain data associated with the sample number of the preceding line; data for individual observations (oxides or elements) must be separated by one or more spaces. The program reads data in floating point or base ten exponential notation. Data from many sources (e.g., USGS Denver microprobe, USGS Branch of Central Mineral Resources Kevex multichannel spectrometer, and USGS Branch of Geochemistry) can be prepared in the required input format with the aid of wordprocessing software that allows ASCII file storage. Numerical observations in the input file followed by L (less than, e.g. 0.05L) and data values of zero are written to the output file as $1x10^{-30}$; SAVEWARE AND DATASAVE programs interpret this value as bdl (below detection limit). Blank data fields can be appended at the end of files created by ASCI2DSV. These blank fields can be used to input additional data into the file at a later time using the DATAEDIT module of DATASAVE (Quick, 1988).

Program Operation

To access the program, type ASCI2DSV at the DOS prompt. The message:

```
PROGRAM: ASCI2DSV

Reads ascii files whose first record is number of samples space number of ox-
ides, whose subsequent even numbered records contain sample IDs, and whose sub-
sequent odd numbered records contain data for a series of oxides or elements,
separated by space(s), and writes DATASAVE readable files

Press any key continue
```

is displayed. The program then prompts:

```
Input file name?          Drive (A or B)?
```

for the name and drive designation of an appropriately formatted input file. Next, a three-letter code designation is requested:

```
What is the sample code (3 characters) ??
```

Specification of this code (WRM in the case of the test file ASCI.DAT) will control how each of the numerical observations in the input file will be assigned to the appropriate oxide/element identifier in the output file. Then the number of oxides/elements in the input file is displayed on the monitor:

```
YOUR INPUT FILE CONTAINS DATA FOR  X       OXIDES/ELEMENTS
```

using the number (X) specified by the second entry on the first line of the input file and prompts with:

```
DO YOU WANT TO APPEND ADDITIONAL OXIDES TO THE INPUT DATA (Y/N) ?
```

If yes (Y), the prompt:

```
HOW MANY ADDITIONAL OXIDES ?
```

solicits input concerning the number of fields to be appended. In order for the data assignment process to proceed properly the number of oxides/elements per sample in the input file (plus the number, if any, of user-defined blank fields to be appended to the input file) must match the number of oxides/elements characteristic of the user-specified code. Similarly, the listing order of oxides/elements in the input file must match the order of elements/ oxides characteristic of the user-specified code.

Storing an output file is the final step; the program prompts:

```
TARGET FILE:                    Drive (A OR B)?
    Default Target File: D:ASCI.WRM
```

The default output file name displayed at the end of the second line of the prompt consists of the root filename of the input file plus an extension equal to the user-specified three letter code assigned to entries in the output file. The default drive for output file storage is the drive from which the input file was read. The defaults are accepted by hitting the ENTER key; they can be overridden by providing a new filename and/or drive designation at the appropriate prompts. Once the output file is stored, the program inquires:

```
PROCESS ANOTHER FILE ? (Y/N)
```

If yes (Y), the program returns to its beginning; if no (N), operations return to DOS.

DSVECORR

Description

DSVECORR is a program that reads a DATASAVE format data file and computes the correlation coefficient between all pairs of oxides/elements from data in the input file. Test data for this program are in the file CORR.DAT. The equation used to compute the correlation coefficients is

$$R = \frac{\sum_{i=1}^{n} X_{ij} \times X_{ik} - \left(\frac{\sum_{i=1}^{n} X_{ij} \times \sum_{i=1}^{n} X_{ik}}{n} \right)}{\sqrt{\left(\sum_{i=1}^{n} X_{ij}^2 - \frac{\left(\sum_{i=1}^{n} X_{ij} \right)^2}{n} \right) \times \left(\sum_{i=1}^{n} X_{ik}^2 - \frac{\left(\sum_{i=1}^{n} X_{ik} \right)^2}{n} \right)}}$$

where n is the number of samples and X_{ij} and X_{ik} are the i^{th} values of oxide/element X_j and X_k, respectively.

When computation is complete an N x N (where N is the number of oxides/elements in the input file) matrix of correlation coefficients is printed. Oxide/element identifiers are printed as the first row and first column of each matrix. Printed correlation coefficient matrices have maximum widths of 15 columns. If the number of oxides/elements in the input file exceeds 15, the remainder of the matrix columns will be printed beneath the first 15 rows. Instances in which all values for one (or both) of the oxides or elements in an oxide/element pair is zero or below detection limit are denoted by the value -10 in the correlation coefficient matrix.

Program Operation

To access the program, type DSVECORR at the DOS prompt. After selecting R (run program), specify the input file at the appropriate prompts. The program prints the name of the file from which the input data was derived, calculates and prints the correlation coefficient matrix, and then displays the initial menu.

DSVEEDIL

Description

DSVEEDIL is a program that reads a DATASAVE format data file, computes ratios between oxide/element abundances in two user-specified samples (i.e. Rb in sample 1 divided by Rb in sample 2, Sr in sample 1 divided by Sr in sample 2, etc.) and graphically portrays the result of the ratio calculation. Test data for this program are in the file EDIL.DAT. The program was developed to aid evaluation of abundance variations (enrichment/depletion), especially the early/late ratio for zoned ash-flow tuffs, in compositionally zoned igneous units. Data for abundances of Na_2O, MgO, Al_2O_3, SiO_2, P_2O_5, K_2O, CaO, Sc, TiO_2, Cr, MnO, FeO, Co, Ni, Zn, Rb, Sr, Y, Zr, Nb, Sb, Cs, Ba, La, Ce, Nd, Sm, Eu, Gd, Tb, Tm, Yb, Lu, Hf, Ta, Th, and U can be input to this routine.

The ratio of an oxide/element's abundance in the first identified sample divided by that in the second identified sample is portrayed as a vertical bar whose height (Y-axis coordinate) is a value between 0 (the abundance of oxide/element A in the first

sample approaches zero and that in the second sample is a value greater than zero) and 3 (the abundance of oxide/element A in the first sample is three times that in the second). If the abundance values of an oxide/element are nonzero in both the first and second sample, an oxide/element identifier is printed at the appropriate position along the X axis; otherwise no identifier is indicated for that X-axis plot position.

If the ratio of an oxide/element in the two input samples is between 0.995 and 1.005 (i.e., if the abundances for the oxide/element are essentially identical in the selected samples), no vertical bar is drawn but a small circle will be drawn at the Y = 1 baseline at the X-axis position of that oxide/element. If the abundance of an oxide/element in either of the identified samples is below the detection limit or was not determined no vertical bar is drawn for that oxide/element.

Program Operation

To access the program, type DSVEEDIL at the DOS prompt. The message:

```
HAVE YOU LOADED AN EGA PRINT SCREEN ROUTINE? IF NOT, DO SO BEFORE PROCEEDING
HIT ESC TO RETURN TO DOS OR ANY KEY TO CONTINUE
```

is displayed. After selecting R (run program) from the menu, specify input file. After file selection, the message:

```
EARLY AND LATE ANALYSES ARE SELECTED USING THE SCROLLER-STRIKE ANY KEY TO CONTINUE
```

is displayed. Strike any key and use the SCROLLER to sequentially identify the first (numerator) and second (denominator) samples to be used for the early/late ratio calculation. Hit the Esc key to exit from the SCROLLER and the message:

```
ADJUST PAPER BEFORE KEYING PrtSc FOR HARDCOPY
```

scrolls the monitor before graphical presentation of the ratio calculation ensues. If desired, hit Print Screen (an EGA print screen routine must be RAM resident) to print a copy of the graph; hit any key to return to the initial menu.

DSVEFELD

Description

The program DSVEFELD reads DATASAVE format data files that contain composition data for feldspars and computes various mineralogic parameters. Test data for this program are in the file FELD.DAT. DSVEFELD has two main branches. One calculates proportions of the anorthite, albite, orthoclase, and celsian feldspar end members for storage as a DATASAVE format data file. The other uses data for coexisting plagioclase and potassium feldspars to compute crystallization temperatures at a user-specified pressure by a number of different algorithms. The feldspar geothermometer programs of David J. Matty (Central

Michigan University) and Fuhrman and Lindsley (1988) were used as the starting point for development of this program; calculations made by DSVEFELD are entirely dependent on algorithms developed by those individuals. DSVEFELD outputs all of the statistics described below to the printer. Printer output is setup to print two sets of calculations per page.

The expected input for this program is rigidly defined. Data for computation and storage of feldspar end member proportions are derived from data file entries whose codes are FSA (plagioclase) or FSK (potassium feldspar). The FSA code has the following oxide identifiers:

K2OA CAOA FE2OA SIO2A AL2OA NA2OA

The FSK code has the following oxide identifiers:

K2OK CAOK FE2OK SIO2K AL2OK NA2OK

Data for geothermometric calculations, based on data for coexisting plagioclase and potassium feldspar, compose a single entry in the data file. Data files should contain samples whose code is FST. The FST code has the following oxide identifiers:
K2OA CAOA FE2OA SIO2A AL2OA NA2OA K2OK CAOK FE2OK SIO2K AL2OK NA2OK
where the first six identifiers, those ending in A, correspond to data for the indicated oxides in plagioclase and the second six identifiers, those ending in K, correspond to data for the indicated oxides in potassium feldspar. Note that the codes FSA, FSK, and FST could also include the identifiers BAOA and BAOK if barium abundances were determined. Note also that iron should be expressed as ferric iron in data files.

Files that contain entries with data for both feldspar species in a single sample can be generated using the BLEND routine in DATASAVE (Quick, 1988). For instance, BLEND can read two data files, one containing data for plagioclase (whose entries have the FSA sample code and contain the oxide identifiers above that end in A) and a second containing data for coexisting potassium feldspar (whose entries have the FSK sample code and contain the oxide identifiers above that end in K) and combine the data from the two input files to form a third file that contains all of the data from the two input files to produce a file whose entries have the FST code and contain all of the oxide identifiers indicated above.

Feldspar end member proportions are calculated using the procedure outlined by Deer and others (1966). End member proportions are written to a file whose entries have the code FEM, which contains the identifiers AB, OR, AN, AND CS for the albite, orthoclase, anorthite, and celsian end members, respectively.

Before calculating crystallization temperatures from data for coexisting plagioclase and potassium feldspar the program computes several mineralogic parameters from the input data. Oxide weight percents are used to compute formula proportions (based on 8 oxygens) for each of the two feldspar species. This data is in turn used to compute X and Z which are sums for alkali metal and tetrahedral site occupancies, respectively. The approach of values for these parameters to ideal values (1 and 4, respectively) provide some indication of analytical data quality. Next, feldspar

end member proportions are calculated for each of the feldspar species.

Feldspar geothermometric calculations constitute the final computation stage in program execution. DSVEFELD computes temperatures using four different algorithms. These algorithms are the general model (equation 28) of Price (1985), equation 5 of Haselton and others (1983), the disordered (sanidine) model of Whitney and Stormer (1977), and the iterative process of Fuhrman and Lindsley (1988). As part of the Fuhrman and Lindsley calculation several other statistics are computed. Their sum of differences provides another indication of input data quality. Feldspar compositions used in their final solution are computed since the iterative process allows the actual input data to be modified within bounds of presumed analytical uncertainty. To more fully understand the calculation process and the import of values computed by the iterative process consult the program description presented by Fuhrman and Lindsley (1988).

Program Operation

To access the program, type DSVEFELD at the DOS prompt. After selecting R (run program) and before specifying an input file the question:

```
COMPUTE AND STORE FELDSPAR END MEMBERS OR DO FELDSPAR GEOTHERMOMETRY (E/T) ?
```

is displayed. Depending on the response to this query, computation of feldspar end members (E) or geothermometric (T) calculations follow input file specification.

If end member calculation was selected, the message:

```
FELDSPAR END MEMBER STORAGE ROUTINE IS OPERATIONAL ONLY IF INPUT DATA FILE
CONTAINS DATA FOR A SINGLE (UNBLENDED) FELDSPAR SPECIES; DOES NOT CALCULATE
TEMPERATURES

HIT ANY KEY TO CONTINUE
```

is displayed. Proceed to the file, drive, and sample specification procedure; select only those samples with FSA or FSK codes from the test file. When feldspar end member computation is complete, output file storage ensues; the program prompts:

```
Fspr target file:                    Drive (A OR B)?
      Default FELSPR FILE: D:FELD.FEM
```

The default output file name displayed at the end of the second line of the prompt consists of the drive from which input data was read, the root filename of the input file, and the extension FEM, which is keyed to the code designation assigned to entries in the output file. The default drive for output file storage is the drive from which the input file was read. The defaults are accepted by hitting the ENTER key; they can be overridden by providing a new filename and/or drive designation at the appropriate prompts. Once the output file is stored, operation returns to the initial menu.

If the feldspar geothermometric option was selected (T), DSVEFELD computes temperatures at the user-specified pressure derived from the response to the query:

```
PRESSURE (IN KBAR) FOR THESE CALCULATIONS =
```

and from data specified in response to the file, drive, and sample identification prompts. The message:

```
WORKING
```

is displayed until the iterative computation process is complete, at which point output is printed and the next set of computations begins. When all of the selected samples have been processed, operations return to the main menu.

DSVEGARN

Description

The program DSVEGARN reads DATASAVE format data files containing composition data for garnets and recasts the data into relative amounts of the six common garnet end members (almandine, spessartine, pyrope, andradite, grossular, and uvarovite) using the algorithm of Rickwood (1968); end member proportions can be stored as a DATASAVE format data file. Test data for this program are in the file GARN.DAT. The program was specifically developed to process garnet composition data obtained by electron microprobe analysis. The input file should contain data for SiO_2, TiO_2, Al_2O_3, Cr_2O_3, MgO, CaO, MnO, Fe_2O_3 and FeO.

In most cases, because the ferric/ferrous ratio of iron in garnets is not known, accurate end-member calculation (specifically, the partitioning of iron between almandine and andradite) is not possible. DSVEGARN includes an option to partition total iron to FeO and Fe_2O_3 assuming ideal stoichiometry; total iron must be expressed as FeO in the input file. Si and an amount of Al sufficient to fill the tetrahedral site are computed. All remaining Al plus Cr and Ti are assigned to the octahedral site and an octahedral site occupancy deficiency is calculated assuming ideal site filling. An iterative loop progressively fills the octahedral site with Fe^{3+} by converting some total iron (FeO) to Fe_2O_3; when the octahedral site is full excess iron remains as FeO. The abundances of Fe_2O_3 and FeO are back calculated from computed Fe^{3+} and Fe^{2+}, respectively.

Output from the end member calculation is printed. A listing of initial oxide abundances is followed by a column in which back calculated FeO and Fe_2O_3 and a new total are printed. The third printed column lists formula atom abundances calculated for a 12 oxygen atom formula. The stepwise assignment of cation atoms to particular garnet end members is presented in a printed table whose righthand column summarizes residuals that remain at the end of the process. Garnet end member mole percents are printed as the last line of the output table.

Calculated end member proportions can also be stored on disk. The output file will have the code GEM associated with each entry. The GEM code includes the identifiers UVAR, ANDR, PYR, SPES, GROS, and ALM (to identify the six common garnet end members) and X (a blank field). The blank field can be edited using DATAEDIT (Quick, 1988) to contain, for instance, the X-coordinate of the electron microprobe stage. DATAPLOT (Quick, 1988) can then be used to plot, for instance, the SPES component abundance variation with position along an X-axis traverse across a garnet grain.

Several conditions may cause the iterative loop to fail. If the octahedral site is filled (or overfilled) by Al, Ti and Cr then none of the total iron is converted to Fe_2O_3, which precludes calculation of any andradite. This condition causes the message:

```
R3+ SITE CONTAINS AN EXCESS - CALCULATION OF FE2O3 NOT POSSIBLE
```

to be printed. If computed FeO is less than 0.009 weight percent the message:

```
COMPUTED FEO IS LESS THAN .009
```

will be printed. If computed Fe_2O_3 is less than 0.009 weight percent the message:

```
COMPUTED FE2O3 IS LESS THAN .009
```

will be printed.

Program Operation

To access the program, type DSVEGARN at the DOS prompt. After selecting R (run program) and before specifying an input file the question:

```
DO YOU WANT TO COMPUTE STOICHIOMETRIC FE2 AND FE3 FROM THE DATA? (Y/N)
```

is displayed and is followed by the question:

```
Do you want to store garnet end member components? (Y/N)
```

The response to the first query determines whether end member computation uses the iterative iron assignment procedure or continues using unmodified input data. Program execution continues following file specification; the message:

```
COMPUTING - STANDBY
```

is displayed during iteration and values calculated for each selected sample are printed. If the second query (above) was answered yes (Y), computed garnet end member abundances will be stored in accordance with answers to the prompts:

```
END MEMBER FILE?                    Drive (A OR B)?
      Default Target File: D:GARN.GEM
```

The default output file name displayed at the end of the second line of the prompt consists of the root filename of the input file

plus the extension GEM (garnet end member), which is keyed to the code designation assigned to entries in the output file. The default drive for output file storage is the drive from the input file was read. The defaults are accepted by hitting the ENTER key; they can be overridden by providing a new filename and/or drive designation at the appropriate prompts. Once the output file is stored, operations return to the initial menu.

DSVEMICA

Description

The program DSVEMICA reads DATASAVE format data files that contain composition data for micas and, using the methodology outlined by Foster (1960a; p. 13-15), calculates mineral structural formulae and a number of mineralogic parameters; cation abundances can be stored as a DATASAVE format data file. Test data for this program are in the file MICA.DAT. The structural formula calculation scheme of Foster precludes computation of anion abundances. These can be calculated separately using DSVEMINF (described below).

DSVEMICA was specifically developed to process mica composition data obtained by a combination of electron microprobe analysis and wet chemical methods. The input file should contain data for as full a subset of the following oxide list as is possible in order to facilitate calculation of the most meaningful structural formula: SiO_2, Al_2O_3, TiO_2, Fe_2O_3, FeO, Li_2O, MnO, MgO, SnO_2, ZnO, P_2O_5, ZrO_2, Cr_2O_3, NiO, CaO, Na_2O, K_2O, BaO, SrO, Rb_2O Cs_2O, H_2O, F, and Cl.

Output from the structural formula calculation is printed. A listing of initial oxide abundances (including an analysis total [TOTAL] and a total adjusted for F and Cl [TOTALa], Deer and others, 1966; p. 516-517) in the analyzed sample is followed by a column that lists formula atom abundances calculated for a 24 oxygen atom formula. A series of half-cell statistics including, tetrahedral, octahedral, and interlayer site occupancies; charges on the tetrahedral, octahedral, and composite layers as well as the interlayer cationic charge; and the lithium-aluminum replacement ratio are printed. For a more thorough discussion concerning the significance of these statistics see Foster (1960a and b). The final piece of printed output for each analyzed mica is a half-cell structural formula.

Cation abundances calculated by DSVEMICA can be stored on disk. The output file will have the code CAT associated with each entry. The CAT code includes the identifiers SI, AL (total aluminum), AL4 (octahedral aluminum), TI, FE3, FE2, LI, MN, MG, SN, ZN, AND NA. DATAPLOT (Quick, 1988) can then be used to plot any combination of these cation abundances on orthogonal, ternary, or histogram plots.

Program Operation

To access the program, type DSVEMICA at the DOS prompt. After selecting R (run program) and before specifying an input file the question:

```
DO YOU WANT TO STORE COMPUTED CATIONS?(Y/N)
```

is displayed. Program execution continues following file specification and values calculated for each selected sample are printed. If the above query was answered yes (Y), computed mica cation abundances will be stored in accordance with answers to the prompt:

```
CATION FILE:                    Drive (A OR B)?
    Default Target File: D:MICA.CAT
```

The default output file name displayed at the end of the second line of the prompt consists of the root filename of the input file plus the extension CAT (cation), which is keyed to the code designation assigned to entries in the output file. The default drive for output file storage is the drive from which the input file was read. The defaults are accepted by hitting the ENTER key; they can be overridden by providing a new filename and/or drive designation at the appropriate prompts. Once the output file is stored, operations return to the initial menu.

DSVEMINF

Description

The program DSVEMINF reads DATASAVE format data files, prompts for a number of oxygens, and calculates generic mineral structural formulae using guidelines specified by Deer and others (1966; p. 515-517). Test data for this program are in the file MINF.DAT. Data for any subset of the oxides SiO_2, Al_2O_3, TiO_2, Cr_2O_3, Fe_2O_3, FeO, NiO, MnO, MgO, CaO, Na_2O, K_2O, P_2O_5, ZrO_2, ZnO, SnO_2, Li_2O, BaO, SrO, Rb_2O Cs_2O, H_2O^+ (chemically bonded water, i.e. OH), F, and Cl can be included in the input file.

Output from the structural formula calculation is printed. A listing of initial oxide abundances (including an analysis total, TOTALa, adjusted for F and Cl, Deer and others, 1966; p. 516-517) in the analyzed sample is followed by a column that lists formula atom abundances calculated for a user-defined number of oxygen atoms in the structural formula.

Program Operation

To access the program, type DSVEMINF at the DOS prompt. After selecting R (run program) and specifying an input file the prompt:

```
ENTER NUMBER OF OXYGENS FOR FORMULA ATOM NORMALIZATION:
```

is displayed. Enter a mineralogically appropriate (Deer and others, 1966) value (24 in the case of the test file MINF.DAT). Calculated structural formulas for each selected sample are

printed. Once the computation and printing are complete operations return to the initial menu.

DSVEREPL

Description

The program DSVEREPL reads DATASAVE format data files that contain abundances for the rare earth elements (REE), prints REE abundances, calculates and prints chondrite normalized abundances, and displays printable EGA chondrite-normalized REE patterns. Test data for this program are in the file REPL.DAT. Data for abundances of La, Ce, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, and Lu can be input to this routine. Output for selected samples can be printed (plotted) individually or in user-specified groups.

DSVEREPL includes two main branches. The first branch computes (and plots) chondrite normalized abundances from input data using an internal set of chondrite normalization values. The default chondrite normalization values are derived from C1 chondrite values of Anders and Ebiharra (1982). Their chondrite abundances have been multiplied by 1.32 to normalize them to a datum that allows their comparison to terrestrial geologic materials. Normalization is required because their C1 chondrite includes excess abundances of volatile components not characteristic of bulk earth chondritic compositions.

The second branch, which is composed of two subbranches, computes (and plots) chondrite normalized abundances from user-specified chondrite normalization values. The first subbranch prompts for a new set of chondrite normalization values whereas, the second subbranch prompts for input necessary to compute (and plot) mineral/matrix (distribution coefficient) REE patterns.

Printed output lists input REE abundances (including a value for the sum of the REE) and chondrite normalized abundances (including a value for the slope of the pattern, i.e. chondrite normalized La/Lu). Chondrite normalized REE patterns are displayed on the monitor and can be printed using Print Screen; an EGA-compatible graphics print screen routine must be RAM resident. The Y axis on the chondrite normalized patterns is logarithmic; values between 0.1 and 10000 times chondrite can be displayed. REE identifiers are printed at appropriate plot positions along the X axis only if the data file contains nonzero values for that particular REE. If the value of an REE abundance is nonvalid, i.e. below detection limit (bdl), not analyzed, or zero, the chondrite normalized REE pattern line is drawn between the previous and the next valid chondrite normalized abundances.

DSVCREPL is an identical program that displays printable CGA chondrite-normalized rare earth element patterns. A CGA print screen routine must be RAM resident.

Program Operation

To access the program, type DSVEREPL at the DOS prompt. The message:

```
HAVE YOU LOADED AN EGA PRINT SCREEN ROUTINE??- IF NOT DO SO BEFORE PROCEEDING
HIT ESC TO RETURN TO DOS OR ANY KEY TO CONTINUE
```

is displayed. After selecting R (run program) and before specifying an input file a series of questions are displayed:

```
DO YOU WANT TO PLOT SELECTED ANALYSES SINGLY OR AS A GROUP (S/G)?
```

Answering single (S) causes each selected analysis to be processed separately; computation and printing of chondrite normalized abundances and plotting of REE patterns proceed one sample at a time. Answering group (G) causes all selected analyses to be processed as a group; computation and printing of chondrite normalized abundances and plotting of REE patterns are completed concurrently for the entire group.

Next, the question:

```
DO YOU WANT TO USE THE DEFAULT CHONDRITE NORMALIZATION VALUES?(Y/N)
```

is displayed. If the answer to this question is yes (Y), operation proceeds to the file and drive designation procedure. Subsequently, REE and chondrite normalized abundances are printed and the message:

```
ADJUST PAPER BEFORE KEYING PrtSc FOR HARDCOPY
```

scrolls the monitor before chondrite normalized REE patterns are displayed. If desired, displayed REE patterns can be printed by hitting Print Screen; after data for all selected samples has been processed hit any key to return to the main menu.

To enable specification of new normalization values, answer no (N) to the preceding question. The question:

```
INPUT NEW CHONDRITE VALUES (C) OR PLOT MINERAL/MATRIX VALUES (M) ?(C/M)
```

is displayed. After answering this question program execution continues to the file specification procedure.

To enable input of new chondrite normalization values hit the C key; the message:

```
ENTER NEW CHONDRITE VALUES
NORMALIZE NEW CHONDRITE VALUES TO APPROPRIATE VALUES BEFORE ENTRY
```

is displayed and a series of prompts facilitate input of these values. Type the numeric value (in parts per million) for the desired normalization value and hit the Enter key at the question mark beneath each successive REE prompt. (See discussion above concerning modification of the Anders and Ebiharra (1982) chondrite to appropriate terrestrial datum). If no normalization value is available for a particular REE, hit the ENTER key. User-defined normalization values are retained by the computer and are used in subsequent program executions until use of default normalization

values or plotting mineral/matrix REE values is specified. After specifying new normalization values, REE and chondrite normalized abundances are printed and the message:

ADJUST PAPER BEFORE KEYING PrtSc FOR HARDCOPY

scrolls the monitor before chondrite normalized REE patterns are displayed. If desired, displayed REE patterns can be printed by hitting Print Screen; after all selected samples have been processed hit any key to return to the main menu.

If the mineral/matrix calculation option (M) was selected, following file and sample specification procedures a series of prompts request information necessary to perform the calculation. The prompt:

ENTER MODAL FRACTION OF MINERAL AS 0.XX

is displayed. If your sample contains 15 percent of the mineral of interest then type 0.15 and hit the Enter key. Then the prompt:

ENTER REE ABUNDANCES IN THE ROCK THAT CONTAINS THE MINERAL

initiates a series of prompts for input of the REE in the rock to which mineral REE abundances will be ratioed. Type the numeric value (in parts per million) and hit the Enter key at the question mark beneath each successive REE prompt. After inputing the required data, mineral REE and mineral/matrix values are printed and the message:

ADJUST PAPER BEFORE KEYING PrtSc FOR HARDCOPY

scrolls the monitor before chondrite mineral/matrix REE patterns are displayed. If desired, displayed REE patterns can be printed by hitting Print Screen; after data for all selected samples has been processed hit any key to return to the main menu.

DSVCREPL operates in an entirely analogous fashion and requires that GRAPHICS.COM be RAM resident.

DSVERGRS

Description

DSVERGRS is a program that reads a DATASAVE format data file and computes statistics for data in the input file. Test data for this program are in the file RGRS.DAT; the file RBVSR.SUB is a subroutine to be used in conjunction with the test data. The program computes a linear regression for the equation:

$$Y = MX + B$$

and computes values for M (slope), B (Y-intercept), and R (correlation coefficient). Linear regressions are computed from user-specified arithmetic expressions that provide derivative definitions for the X and Y axes. For instance, if the input data file contains data for Zr, Nb, Rb and Sr statistics can be calculated for Rb (X axis) versus Sr (Y axis) or for the more complex axis definitions Zr/Nb (Y axis) versus Rb + Sr (X axis). All X and Y

axis definitions are specified using subroutines that are similar to those used by DATAPLOT (Quick, 1988) to generate plots. These subroutines can be written as part of running DSVERGRS. A graphical portrayal of the input data, calculated regression line, and statistical parameters are displayed on the monitor and can be output to a printer using Print Screen. Monitor output can be displayed on either CGA or EGA systems; a compatible graphics Print Screen routine must be RAM resident to enable transmission of the monitor image to a printer.

Program Operation

To access the program, type DSVERGRS at the DOS prompt. The program displays the message:

```
HAVE YOU LOADED AN EGA PRINT SCREEN ROUTINE?
IF NOT, DO SO BEFORE PROCEEDING
HIT ESC TO RETURN TO DOS OR ANY KEY TO CONTINUE
```

The initial menu for DSVERGRS:

```
                    PROGRAM: DSVERGRS
********************  MENU  **********************
D    Directory                E    Edit Subroutine
S    Sample Code File         R    Do Regression
                   ESC   Exit Program
***************************************************
        Sample Code File:   CODES
        Current Data File:
        Current Subroutine:
```

is slightly different than other SAVEWARE program menus because this program operates somewhat differently. Select D to see a directory for a user-specified drive. Select S to select a sample code file appropriate to the data that will be processed. Select E to edit a subroutine. The Edit Subroutine menu is displayed:

```
******* STACK EDITOR *******
Your choices are as follows:
 N    Make a New Subroutine
 E    Edit an old subroutine
ESC   Exit to initial menu
```

Select N to create a new subroutine or E to edit an old subroutine, as appropriate. The procedure for creating or editing axis definition subroutines is fully documented by Quick (1988) and is not further described here.

Now that an appropriate subroutine (e.g. RBVSR.SUB on disk 2), that specifies the functions that appropriately define the X and Y axes, exists (having been written using DATAPLOT or in earlier sessions using DSVERGRS) select R to begin the regression computation process. Supply answers to the prompts:

```
Subroutine name?          Drive (A or B)?
Data file name?           Drive (A or B)?
```

as appropriate. When specifying the subroutine file, type the filename without the .SUB extension, DSVERGRS automatically supplies this part of the file designation. The screen is cleared

and a summary of information concerning the selected file and three additional prompts are presented:

```
There are 4 samples in the file.
  Sample code       # of samples
      ALL               4
      Use this file (Y/N)?
      List values (Y/N)
      Plot all data (Y/N)
```

Answer yes (Y) to the first question to verify the selected file or no (N) to return to the file specification procedure. Answer yes (Y) to the second question to have values calculated by the axis definition subroutine printed or no (N) to suppress this feature. Answer yes (Y) to the third question to use all of the data in the specified input file or no (N) to enter the SCROLLER routine described in then General Comments section. After the input data has been processed by the axis definition subroutine, the prompt:

```
Recall more data (Y/N)?
```

is displayed. Answer yes (Y) to recall more data or no (N) to proceed with the regression computation. If more data is to be recalled, program execution returns to the file specification procedure. Once sample selection is complete a summary of statistics, including the number samples (N) selected from the input file; mean, maxima, and minima values for X and Y; and slope (M), Y-intercept (B), and correlation coefficient for the calculated regression line are displayed on the monitor. This data can be printed by hitting the Print Screen key. The prompt:

```
DO YOU WANT TO SEE THE FIT GRAPHICALLY?(Y/N):
```

is displayed beneath the statistical summary. Answer yes (Y) to plot the data and regression line on the monitor or no (N) to return to the initial menu. If a graphical portrayal is requested the prompt:

```
ENTER STARTING X,TICK MARK SPACING,FINAL X
```

will be displayed. Enter three values (separated by commas) that bound the minimum X value, indicate a desired tick mark spacing along the X axis, and bound the maximum value for X, respectively. Then the prompt:

```
ENTER STARTING Y,TICK MARK SPACING,FINAL Y
```

will be displayed.
Enter three values (separated by commas) that bound the minimum Y value, indicate a desired tick mark spacing along the Y axis, and bound the maximum value for Y, respectively. The program then prompts:

```
CGA OR EGA? (C/E):
```

to determine the type of monitor that is being used. Enter C to specify a CGA monitor and E to specify an EGA monitor. A final message is displayed:

```
INPUT DATA AND REGRESSION LINE WILL BE DISPLAYED ON MONITOR
HIT PRINT SCREEN TO TRANSMIT SCREEN IMAGE TO PRINTER
WHEN PRINTING IS COMPLETE, HIT ANY KEY TO CONTINUE

HIT ANY KEY TO CONTINUE
```

At this point the monitor clears. The input data, regression line, and specified tick marks are plotted on the monitor; values for Y-intercept (B), slope (M), and correlation coefficient (R) are displayed beneath the plot. If desired, hit Print Screen to transmit the screen image to the printer; hit any other key to display the initial menu.

DSVESPDR

Description

The program DSVESPDR reads a DATASAVE format data file that contains abundances for a number of trace elements, prints trace element abundances, calculates and prints chondrite normalized abundances, and displays a printable EGA graph that portrays chondrite-normalized extended trace element patterns. Test data for this program are in the file SPDR.DAT. Data for abundances of Rb, Ba, Th, K_2O, Nb, Ta, La, Ce, Sr, Nd, P_2O_5, Sm, Zr, Hf, TiO_2, Tb, Y, Tm, and Yb can be input to this routine; the program converts weight percent data for K_2O, P_2O_5, and TiO_2 to parts per million of the element. Output for selected samples can be printed (plotted) individually or in user-specified groups.

Chondrite normalization values are those of Thompson and others (1983). Printed output presents input and chondrite normalized trace element abundances. Chondrite normalized patterns are displayed on the monitor and can be printed using Print Screen; an EGA-compatible graphics print screen routine must be RAM resident. The Y axis on the chondrite normalized patterns is logarithmic; values between 0.1 and 1000 times chondrite can be displayed. Trace element identifiers are displayed at appropriate plot positions along the X axis only if the data file contains nonzero values for that particular element. If the value of an element abundance is nonvalid, i.e. below detection limit (bdl), not analyzed, or zero, the chondrite normalized pattern line is drawn between the previous and the next valid chondrite normalized abundances.

DSVCSPDR is an identical program that displays printable CGA chondrite-normalized extended trace element patterns. A CGA print screen routine must be RAM resident.

Program Operation

To access the program, type DSVESPDR at the DOS prompt. The messages:

```
PROGRAM EXPECTS TIO2, P2O5, AND K2O AS WEIGHT PERCENTS (CONVERTS THEM TO PPM);
EXPECTS ALL OTHER ELEMENTS AS PPM

HAVE YOU LOADED EGAEPSON.COM? IF NOT, DO SO BEFORE RUNNING PROGRAM TO ENABLE
PRINT SCREEN.      HIT ESC TO RETURN TO DOS OR ANY KEY TO CONTINUE
```

are displayed. After selecting R (run program) and before specifying an input file the question:

```
DO YOU WANT TO PLOT SELECTED ANALYSES SINGLY OR AS A GROUP (S/G) ?
```

is displayed. Answer single (S) if selected analyses are to be processed separately; computation and printing of chondrite normalized abundances and plotting of chondrite-normalized patterns proceed one sample at a time. Answer group (G) if all selected analyses are to be processed as a group; computation and printing of chondrite normalized abundances and plotting of chondrite-normalized patterns are completed concurrently for the entire group.

Following file and sample specification, trace element and chondrite normalized abundances are printed and the message:

```
ADJUST PAPER BEFORE KEYING PrtSc FOR HARDCOPY
```

scrolls the monitor before chondrite normalized patterns are displayed. If desired, displayed patterns can be printed by hitting Print Screen; after data for all selected samples has been processed hit any key to return to the main menu.

DSVCSPDR operates in an entirely analogous fashion and requires that GRAPHICS.COM be RAM resident.

DSVEWALK

Description

The program DSVEWALK reads DATASAVE format data files that contain major oxide abundances for basalt samples; original data may be modified to reflect the effect of adding or removing olivine and (or) plagioclase of specified compositions. Test data for this program are in the file WALK.DAT. DSVEWALK calculates several sets of plot coordinates and displays a plot that portrays compositions of basalts projected onto the diopside-olivine-silica saturation surface of the simplified basalt phase system using the methods of Walker and others (1979) and Pallister (1987). The monitor image can be transmitted to a printer using Print Screen; a CGA-compatible Print Screen routine must be RAM resident.

The compositions of plagioclase and olivine used to modify input data are given below:

	Plagioclase	Olivine
SiO_2	49.97	40.73
Al_2O_3	31.66	0.08
FeO	0.44	9.12
MgO	0.00	48.83
CaO	15.62	0.00
Na_2O	2.79	0.00
MnO	0.00	0.07

Any amount, between -100 and +100 percent, of any combination of these minerals can be added or subtracted from the samples whose compositions are being evaluated to test for the effects of mineral fractionation or accumulation. Input a positive percentage if the mineral is inferred to have been fractionated from or a negative percentage if the mineral is inferred to have accumulated in the sample whose composition is being evaluated. Input percentages indicate the bulk fraction to be accounted for by the specified mineral, whereas the remainder of the bulk fraction indicates the contribution of the sample whose composition is being evaluated. For instance, if it is hypothesized that 15 percent of a sample is accumulated plagioclase (and it is deemed necessary to remove this effect before comparing the whole rock composition to those in the experimental basalt system) then one would opt to subtract 15 percent plagioclase from the input analysis.

DSVEWALK prints results of ternary proportion calculations. The first line of the output indicates the sample number, the percentages of olivine and or plagioclase, if any, that were added to (or subtracted from) the input, and the sum of SiO_2, Al_2O_3, FeO, Fe_2O_3, MnO, MgO, CaO, Na_2O, and K_2O in the input analysis. The next two blocks of printed output indicate plot coordinates as computed by Walker and others (1979) and as transformed, ternary plot coordinates.

Program Operation

To access the program, type DSVEWALK at the DOS prompt. The message:

```
HAVE YOU LOADED A CGA PRINT SCREEN ROUTINE?
IF NOT, DO SO BEFORE PROCEEDING
HIT Esc TO RETURN TO DOS OR ANY KEY TO CONTINUE
```

is displayed. After selecting R (run program) and following file, drive, and sample specification the message:

```
SAMPLE:XXXXXXXXXXXX
```

where XXXXXXXXXXXX is the identity of the sample whose data is being processed, is displayed. That message is followed by the sequentially displayed prompts:

```
ENTER %OL TO BE ADDED (-100 TO 100%)
ENTER %PL TO BE ADDED (-100 TO 100%)
```

Enter olivine and (or) plagioclase abundances hypothesized to have been removed or added, or hit ENTER to indicate that no addition or subtraction, respectively, of these phases is desired prior to computation. When these values have been entered for all selected samples, computation and results printing follow. At the completion of printing the monitor scrolls the message:

```
AFTER PrtSc..PUSH ANY KEY TO CONTINUE
```

and then displays a plot of the selected sample compositions projected onto the diopside-olivine-silica saturation surface of

the simplified basalt phase system. If desired, the plot can be directed to the printer by hitting Print Screen; hit any key to return to the initial menu.

DSVFEWAT

Description

The program DSVFEWAT reads DATASAVE format data files that contain major oxide abundances for rock samples and recalculates analyses to 100 percent, anhydrous. Test data for this program are in the file FEWAT.DAT. The program also allows iron to be partitioned between FeO and Fe_2O_3 in various ways. Recalculated analyses can be stored as DATASAVE format data files. TiO_2 and K_2O abundances are recalculated to parts per million of the elements. A summary of all recalculations is printed in tabular form.

In many cases it is meaningful or helpful to normalize major oxide analyses to 100 percent on an anhydrous basis. The first branch of DSVFEWAT normalizes data accordingly and stores a data file that contains the modified data. Whether this option or the storage option that follows iron partitioning (described below) is selected a new data file will be written whose entries have the WRM code and include modified abundances of SiO_2, Al_2O_3, Fe_2O_3, FeO, MgO, CaO, Na_2O, K_2O, TiO_2, P_2O_5, MnO, and H2O; analyses total 100 percent, discounting H_2O. If oxide data in the input file includes associated standard deviations (as might be the case for a file that contains computed average compositions), the standard deviations are also multiplied by the factor used to normalize the oxide abundances.

Many major oxide analyses report total iron as Fe_2O_3. It may be necessary, as in the case of normative mineral calculations, to partition total iron to FeO and Fe_2O_3. DSVFEWAT allows iron to be partitioned in two ways. It can be partitioned according to the guideline of Irvine and Baragar (1971) whereby Fe_2O_3 is limited to the value, expressed in weight percent, TiO_2 + 1.5; all remaining iron is recast as FeO. Alternatively, the molecular abundance of FeO to total iron expressed as FeO can be set to some value. DSVFEWAT can modify data in either fashion and stores derivative data. The program automatically computes FeO and Fe_2O_3 from total iron expressed as Fe_2O_3 and FeO determined by wet chemistry, if the latter is present in the input file. After iron partitioning a second opportunity to normalize analyses to 100 percent on an anhydrous basis is presented. Data will be stored as described above.

Parts per million values of Ti and K are required for some petrogenetic studies or plots. DSVFEWAT computes and prints these values from input files.

Program Operation

To access the program, type DSVFEWAT at the DOS prompt. After file, drive, and sample specification, the message:

```
PROGRAM EXPECTS TO READ A DATA FILE CONTAINING TOTAL IRON AS FE2O3 AND FEO
(FERROUS IRON)--YOU WILL HAVE AN OPPORTUNITY BELOW TO RECOMPUTE TOTAL IRON AS
FE2O3 IF IT HAS ALREADY BEEN PARTITIONED TO FE2O3 AND FEO
```

is displayed. The question:

```
RECALCULATE ANALYSES TO 100%, ANHYDROUS, STORE DATA, AND EXIT (Y/N)?
```

follows. If this is the desired result, answer yes (Y). Computed oxide abundances can be stored in accordance with answers to the prompt:

```
NEW MAJORS FILE:                    Drive (A OR B)?
     Default majors file NORMALIZED 100% ANHYDROUS: D:FEWAT.WRM
```

The default output file name displayed at the end of the second line of the prompt consists of the root filename of the input file plus the extension WRM (whole rock majors), which is keyed to the code designation assigned to entries in the output file. The default drive is the drive from which the input file was retrieved. Default file and drive designations are accepted by hitting Enter at the appropriate prompts; otherwise new file and drive designations can be input at the appropriate prompts.

If the answer to the previous question was no (N), the question:

```
COMPUTE AND STORE FE2O3 AND FEO FROM I&B RULE (T) OR FROM
INPUT MOLECULAR FEO/FEOT RATIO (R)--(T/R)?
```

is displayed. If the answer is T, the Irvine and Baragar (1971) guideline described above will be used to partition total iron. If the answer is R, the prompt:

```
ENTER VALUE FOR IRON RATIO
```

will be displayed. A value between 0.00 and 1.00 should be entered. Ringwood (1975) indicates that a value of 0.9 is appropriate for basaltic compositions. The value of FeO/FeOT decreases with increasing silica content though this observation has not been quantified.

The question:

```
IS FE2O3 IN DATA FILE=FE2O3T (T) OR HAS IT BEEN PARTITIONED (P) TO
REAL FE2O3 AND FEO (T/P)?
```

is displayed. If the answer is T, program execution continues, otherwise the values of partitioned iron will be recombined to total iron as Fe_2O_3 before processing continues.
The final prompt:

```
NORMALIZE ANALYSES TO 100% ANHYDROUS BEFORE STORING DATA (Y/N)?
```

is displayed; it provides an opportunity to normalize data after iron has been partitioned but before file storage. Computed oxide abundances can be stored in accordance with answers to the prompt:

```
NEW MAJORS FILE:                    Drive (A OR B)?
     Default majors file with MODIFIED IRON VALUES: D:FEWAT.WRM
```

At this point a table is printed that summarizes recalculated data. The first column includes the sample numbers of all entries chosen for processing. The next block of four columns presents the results of iron partitioning based on a file that contains total iron as Fe_2O_3 and FeO as determined by wet chemistry. The first column in this block indicates values of total iron expressed as Fe_2O_3. The second column presents values of FeO as determined by wet chemistry. The third column presents Fe_2O_3 as computed by difference from total iron as Fe_2O_3 and determined FeO. In making this last calculation, note that an amount of Fe_2O_3 is converted to an equivalent amount of FeO by multiplying weight percent Fe_2O_3 by 0.8998 and that FeO is converted to an equivalent amount of Fe_2O_3 by multiplying weight percent FeO by 1.1114. These factors account for the fact that the molecular weights of FeO and Fe_2O_3 are not the same, i.e the proportion of metallic iron is higher in FeO than it is Fe_2O_3. The fourth column in this block indicates the new value for the analysis total. Converting some Fe_2O_3 to FeO causes the value of the total to decrease.

The third block of columns provides iron partitioning data derived by the chosen method; i.e. the Irvine and Baragar guideline or the user-specified molecular iron ratio. The method used to partition iron is specified above these columns; in the case of the molecular iron ratio method the user-defined value of the ratio itself is printed. The first and second columns in this block are derived by converting all iron to FeO. This value is multiplied by the user-specified molecular iron ratio to give the FeO value. FeO is subtracted from total iron as FeO; this remainder is converted back to Fe_2O_3. The third column gives a total that reflects the effect of iron partitioning, as described above; this total will be 100.00 if the analysis was normalized to 100 percent anhydrous before being stored.

The final two columns simply present the result of converting K_2O and TiO_2 to parts per million of the elements, respectively.

After file storage, as described above, processing returns to the initial menu.

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