DEPARTMENT OF THE INTERIOR

U.S. GEOLOGICAL SURVEY

MINCLC: A FORTRAN program for recalculating mineral analyses

by

W.P. Freeborn, E.S. McGee, and J.S. Huebner

U.S. Geological Survey

OPEN-FILE REPORT 85-257

1985

CONTENTS

TABLES

FIGURES

APPENDICES

MINCLC: A FORTRAN program for recalculating mineral analyses

by

W. P. Freeborn*, E. S. McGee, and J.S. Huebner

ABSTRACT

MINCLC is a generalized FORTRAN program for recalculating chemical analyses of minerals. It accepts weight-percent values for as many as 30 elements from a set of 68 components listed in any order. The program calculates cation formula units and element ratios and can adjust proportions of the species of a multivalent element to achieve a specified cation-to-anion ratio. For pyroxene minerals, the program also calculates formal site occupancies and normative components. Default operating conditions permit the program to function properly for petrologic and mineralogic problems involving most common rock-forming silicates, oxides, sulfides, carbonates, sulfates, phosphates, and nitrates.

INTRODUCTION

MINCLC is a versatile FORTRAN program for converting chemical analyses to mineral formulas. It uses oxide weight-percent values as input and puts out values of oxide weight percent, cations, and cation ratios. Because some chemical analytical techniques, such as electron microprobe analysis, do not differentiate between the reduced and oxidized valence states of an element, the program can perform a redox calculation to estimate the amounts of the reduced and oxidized species of multivalent element. When an oxidation-state change (REDOX) is desired, the current version of MINCLC will vary not only the amount of Fe^{2+}/Fe^{3+}, but also Mn^{2+}/Mn^{3+}, Cr^{2+}/Cr^{3+}, or Ti^{3+}/Ti^{4+}, as needed. After a REDOX calculation, new ratios and, if applicable, new site occupancies and norm components are calculated and printed. The program can recalculate analyses of minerals to any specified number of cations or anions, and if a REDOX is specified, the analysis is recalculated to a specific cation:anion ratio. For pyroxenes (using a 4:6 cation:anion ratio), it will also calculate formal site occupancies and norms. MINCLC is a more general program than the pyroxene end-member program by Ikeda (1979), because it allows for a wider range of pyroxene compositions and more readily varies element redox states. The program is also more general in nature than the program by Smyth (1980), which calculates pyroxene end members and Fe^{2+}/Fe^{3+} ratios. As the program is presented here, an analysis can contain as many as 30 elements, in any order, and the elements used can vary from one analysis to the next. These elements must be selected from a list of 68 components, including all elements that have an atomic number of 30 or less, and 32 additional components of possible geologic interest.

* Now at Materials Research Laboratory, Pennsylvania State University, University Park, PA 16802

BACKGROUND

The program was originally written as Mincalc by Phelps Freeborn for the U.S. Geological Survey's (USGS) IBM 370 computing system and then converted by him to run on the Honeywell 183 computer with Multics operating system. Mincalc was renamed MINCLC when it was modified by J.S. Huebner to run on a Digital Equipment Corporation PDP 11/23 computing system running under the TR-11 operating system with Fortran IV, versions 2.5 and 2.6. The version of the program described here runs in a 64-kB system, using only a very basic FORTRAN compiler. MINCLC is especially useful for users of the USGS Reston Microprobe Facility because analyses stored on floppy disks during microprobe operation can be converted to a format acceptable for input to MINCLC by using the program RDARL4 (Huebner, 1983).

This report provides information on how to run the program, the mathematical techniques used in some of the calculations, and information for programmers interested in the specifics of the program. The section for general users of MINCLC explains the main features, the various options available, and a few qualifications and cautions. Descriptions of the mathematical techniques used in the calculations, such as those for adjusting the redox state of an element, the site occupancy calculation, and the pyroxene norm calculations, are included here because general users of MINCLC should understand the limitations of these calculations. Programmer information is contained in the last section. Topics covered include functions of the various subroutines, a heirarchy for the program, and a list of variables and arrays used. Specialized information on features that probably will be rarely used, such as reordering of the normative calculation or changing the list of elements recognized by the program, is given at the end of the report.

USER INFORMATION

INPUT CHARACTERISTICS

The input file contains directions for running a set of analyses and the data for each analysis. Figure 1 is an example of an input file. The first record, which contains **** as the first 4 characters, is a control record that indicates the options selected and the desired cation:anion ratio. A control record can also be inserted at other places in the file in order to change the options or the cation:anion ratio and can be useful if data for several mineral species are being processed. Table 1 lists the three possible control arguments available (any number of which may follow the four asterisks) and their functions. The two numbers near the end of the ****control record, right-justified in columns 51-60 and 61-70 (Fig. 1), are the desired numbers of anions and cations to be used in calculating the mineral formula. (These anions are assumed to be divalent.)

Sets of records follow the control record, one set for each analysis. Each set consists of a title followed by one to four records of data. The title can contain any ASCII characters, except that it cannot have **** in the first four columns and it must have at least one character other than a blank, decimal point, or numeral in columns 3-8. The next one to four records contain the data for one analysis as pairs of element symbols and weight-percent values, with as many as 9 elements per line for as many as 30 elements listed in any order. Table 2 lists the elements, their valence states, and input information. Elements such as H, F, K, etc., must be coded as a letter followed by a blank. Elements that have variable oxidation states (S, Ti, Cr, Mn, Fe) have been assigned two

or three names that distinguish the oxidation states (Table 2). The table of atomic proportions will be printed with elements listed in the order in which they were input. If an element appears more than once, the first occurrence is used in the calculations. If MINCLC encounters an element that is not listed in Table 2 or is incorrect, the corresponding datum is skipped and a warning is printed. The input format for the element symbols and weight-percent oxides 9(2A,F6.2) is as shown in Figure 1. The list of elements must be terminated with $$ in the element symbol location following the last oxide weight percent or, if a record has 9 elements and concentration values, in position 73 and 74. The occurrence of $$ will prevent the reading of unused data fields or the reading of a title record as data. As many analysis sets as desired can be used in one file. No special terminal record is needed at the end of the file. MINCLC expects most (but not all) concentration values as oxide weight-percent values. The exceptions are He, O, F, Ne, Cl, and Ar (Table 2), which are entered as element weight-percent values.

OUTPUT CHARACTERISTICS

The table shown in Figure 2A may be printed on the header page of the output as a reference for the user, in order to show some of the values used by the program in performing the calculations. The program produces one page of output for each analysis, or two pages if the REDOX subroutine is used. Figure 2B is a sample of the first page of printout from the program, showing most of the options. The input data are printed as they were read so that they can be easily checked for input errors. Weight percent, cation, and anion totals are included as output. Various element ratios are calculated and printed. The pyroxene site occupancies are generated if the desired number of cations is four; pyroxene norm components are generated if the cation:anion ratio is 4:6 and the SiO_2 value is greater than 20 weight percent.

The recalculated analysis (Figure 2B) is twice presented as a list of cations. In the first occurrence, the numbers of cations shown are the numbers of cations associated with corresponding anion numbers that total (are normalized to) the ANION value read in the preceding control record. The second list contains cation numbers normalized to total the value of CATION in the control record. The columns can also contain values for anions (OH, O, F, Cl) that have a negative charge (Table 2). These anion values are not included in the cation totals, but they are used in the anion totals by contributing a value that is equal to their equivalence in divalent oxygen ions (Table 2).

The redox calculation is an option that must be requested in the control arguments, and, if requested, will generate additional output (Figure 2C) showing the recalculated analysis. The "redox" output is similar to that on the first page, but variable oxidation state elements have been added as needed and adjusted in an attempt to achieve the specified anion:cation ratio.

If the redox calculation is used, the program also shows an alternative way of achieving the correct anion:cation ratio solely by adding or subtracting SiO_2. (When Si is not included in the input, this step is omitted.) If the

adjustment in SiO_2 is less than the analytical uncertainty in SiO_2, the result that follows, calculated by adjusting the oxidation states of the elements, is not significant. The redox recalculation should be considered realistically because it assumes only one source of error in the analysis, the determination of the proportions of the oxidized and reduced states of the multivalent elements titanium, chromium, manganese, and iron. The failure to achieve the ideal anion:cation ratio during the recalculation, or the amount of redox adjustment actually made, can actually depend on real imperfections in the data, real deviations of a phase from ideal stoichiometry, or the possibility that two phases having different cation:anion ratio were inadvertently analyzed as one phase. Use of MINCLC is no substitute for independent judgement. For example, one should regard with suspicion a recalculation that converts half the iron to the ferric state in a lunar pyroxene that crystallized under a highly reducing condition. Such an unreasonable redox adjustment would probably result from analytical error.

Usage of MINCLC was intended for, but is not restricted to, silicates and oxides that have a formula based on an oxygen lattice, because oxygen anions are assumed to be associated with positively charged cations so that charge balance is maintained. In two situations, the program has additional flexibility. MINCLC correctly calculates formula units for carbonates, sulfates, and any other compounds based upon a negatively charged radical composed of a cation plus oxygen anions (Figure 2D). MINCLC also correctly calculates formulas in which OH, F, and Cl proxy for oxygen positions. Thus, the program can recalculate analyses of hydrous silicates such as the amphiboles and micas (Figure 2D). The program will not adjust the concentration or amount of (OH + F + Cl) to achieve a desired stoichiometry. Thus, because analyses of H_2O, Cl, and F in silicates are uncertain and prone to error, a user of MINCLC may want to recalculate such silicates on an anhydrous basis. The program will also correctly calculate analyses for sulfides, provided the sulfur in the analysis is labeled with the symbol for the desired valence (S1 or S2, see Table 2).

MATHEMATICAL CONSIDERATIONS

This section is intended to provide some insight into the calculations upon which the results seen by the user are based.

REDOX CALCULATION

The redox calculation, which is done only when RDOX appears in the preceding control record, attempts to minimize the difference between the ideal number of anions (provided as input on the control record) and the calculated sum of the anions in the analysis. The adjustment is made only if the difference in the anion totals is greater than the value of er5, or 0.0005. The program uses twice the difference in the anion totals as the amount of charge (electrons) to be adjusted, and both the oxidized and reduced valences of an element are adjusted. If only one valence state of an element was included in the input, the other state is added to the list if it is needed for the calculations. The multivalent elements that can be adjusted by the current version of the program are: Fe, Mn, Cr, and Ti. The elements are adjusted sequentially, as described below, until the difference in the anion totals is eliminated or all the elements have been adjusted. If the calculation is successful, the cation and anion totals are normalized to the desired values.

When the calculation is complete, new oxide weight percent and cation totals are calculated using the newly determined cation values of the multivalent elements.

The order in which the multivalent elements are adjusted depends on whether an oxidation or a reduction is required. The program determines whether an oxidation or a reduction is to be done by testing whether the deficiency (desired anion minus calculated anions) is positive or negative. For oxidation, the order is Ts->Ti, C2->Cr, Fe->Fc, and Mn->Mc. For reduction, the order would be opposite (Mc->Mn, Fc->Fe, Cr->C2, Ti->Ts). The above order corresponds to the relative redox potentials of the redox couples and makes sense chemically and mineralogically.

Figure 3 shows a sample oxidation calculation to illustrate the procedure used. Figures 2B and C provide the complete analysis. Since Ti and Cr were input in their oxidized valence state, the next element to be adjusted would be Fe. The anion proportions normalized to 4.00 cations are used in the redox calculation because it is the deficiency in the anion total that is being adjusted. Ferric iron will be added as an element in the list (Figure 2C) during this calculation because it was not included in the original input element list (Figure 2B). If the deficiency (def) equals 0 after the iron is adjusted (step 6, Figure 3), then the calculation is complete; if it does not, then the calculation continues at step 3 with the cation value of the next multivalent element (Mn, in this case). If each of the multivalent elements is adjusted and the difference in anion totals is not eliminated, a message is printed, giving the remainder of oxygens after all adjustments.

For a reduction calculation, the procedure followed is similar to that outlined above, except that the deficiency (def) would be a negative number. The cation value of the oxidized element (x) would be tested to see if its value was less than -cor (similar to step 3, Figure 3), and if it was, then cor would be set equal to -cat(x).

ADJUSTMENT OF SILICA

An important feature included with the RDOX option serves as a reminder about the possible significance of the redox calculations. The statement about an adjustment of silica (Figure 2C) is shown with the redox calculation because it is an alternative method to attain the ideal anion:cation ratio. This statement is primarily printed as a warning to emphasize that the apparent need for a change in oxidation state may be due solely to analytical error (Figure 2C). Silica is used in the warning calculation because it is the most abundant component in pyroxenes and most other silicates. (The adjustment is skipped and the statement is not printed if SiO_2 = 0 in the input.) In performing this calculation, the program adjusts the anion:cation ratio solely by adding or subtracting SiO_2 from the analysis. If the required adjustment in SiO_2 is less than the uncertainty in the SiO_2 analysis, the following redox calculation is not likely to be significant. The SiO_2 adjustment is calculated by using:

$$\text{correction} = 2 * (\text{desired anions} - \text{calculated anions})$$

which is the same figure being used in the redox calculation. The relative percent which this represents and the proposed change in silica value are then calculated:

relative percent = 100 * (correction / Si cations)

change wt. % Si = relative percent * wt. % SiO_2

The user must evaluate the information presented from this calculation and the results of the redox calculation.

SITE OCCUPANCY

MINCLC calculates a formal pyroxene site occupancy whenever the desired cation number specified in the preceding control record is 4, the value for a stoichiometric pyroxene with 6 oxygen formula units. The site occupancy calculation is performed by utilizing the cation numbers from the column that totals 4 cations, then filling the three crystallographic sites in the order: tetrahedral site, then eightfold site, and, finally, octahedral site. Elements, shown below, are used in the order listed, from left to right, until the appropriate site is filled.

a. tetrahedral site: Si, Al, Fc, Ti (maximum = 2.000 cations)
b. eightfold site: K, Na, Li, Ca, Mn, Zn, Fe, Mg, Ni (maximum = 1.000 cations)
c. octahedral site: Al, Mg, Fc, Ni, Ti, Cr, Ts, C2, Mc, Fe, Mn, Zn (maximum = 1.000 cations)

The order in which the cations are used is based on crystal-chemical restrictions. No other cations are allowed in the pyroxene sites and the maximum number of cations for any site may not be exceeded. If any cations are not assigned to a site, MINCLC prints their element names and the residual cation number of each that remains unassigned.

The initial normalization of the cations to a sum equal to 4.000 assures that, for analyses of real pyroxenes, each site will appear to be perfectly filled. However, this representation of the site occupancy generally does not assure that the mineral formula has exactly 6.000 oxygens. After a successful redox calculation, the sites will appear perfectly filled and the oxygen sum will be 6.000. MINCLC users should regard the formal site-occupancy calculation with caution; as described above, a redox calculation can make the site-occupancy calculations appear correct. In addition, even if the sum of the anions is close to 6.000 per 4.000 cations, cation vacancies, which occur in some pyroxenes (Robinson, 1980) are assumed by MINCLC not to occur.

PYROXENE NORM

The normative calculation of mineral components, like the CIPW norm for rocks (Cross et al., 1903), provides a reproducible method for naming and describing the mineral species within a mineral group such as pyroxenes. For instance, strong justification for the new pyroxene mineral species donpeacorite (Petersen et al., 1984) is that this pyroxene contains 63% of a single component ($MnMgSi_2O_6$) in the mineral norm. However, to date, there is no universally accepted normative scheme for calculating pyroxene components. MINCLC incorporates a scheme devised by Malcolm Ross of the USGS. An important feature of the program is the ability to reorder or redefine the pyroxene components. If a different scheme of pyroxene normative calculation achieves

universally accepted status in the future, it will be relatively easy to change the MINCLC scheme so that it conforms.

Normative pyroxene components are calculated and printed if the anion to cation ratio is 6:4 and if the SiO_2 value input is greater than 20 wt. %. The calculation technique is like any used in a rock-norm calculation: by following a specified hierarchy, sites are filled on the basis of the smallest amounts of a particular element, until all the elements are used up. MINCLC's pyroxene normative scheme uses a list of 64 different components (Table 3). The components are constructed by filling the M2, M1, and 2 Tetrahedral (T) sites of the pyroxene. In Table 3, the components have been grouped into blocks that are calculated in a similar manner, on the basis of the charges of the cations filling the sites. In the program itself, these groups have been generalized to 6 types, which can be described in the general forms shown in Table 4. Sometimes, as in types 2 and 3, several forms use the same method of calculation.

The pyroxene norm calculation performed by MINCLC differs from Smyth's (1980) procedure in that no components with vacancies are calculated by MINCLC. The default mode of the program uses all recognized major pyroxene components (see Table 3), but 27 possible minor components are omitted from the default calculation. MINCLC includes an option for changing the number and/or the order of the pyroxene components calculated. Instructions for using this option to calculate additional recognized pyroxene components follow the programmers information section. Use of the option does not require any programming skills, but because the utility of a norm calculation lies in following a standard procedure, this feature should be used with discretion.

Any cations that could not be included in the normative calculation are listed in the printout. These values of residual cations may result from imperfections in the analysis or from the real presence of minor normative components that are not included in the default list of components. Alternatively, the residuals may be real, representing deviations from pyroxene stoichiometry.

The normative routine includes a calculation of the proportions of the pyroxene components Wo($CaMgSi_2O_6$), En($Mg_2Si_2O_6$), and Fs($Fe_2Si_2O_6$), according to Wo=($Ca_2Si_2O_6$/($Mg_2Si_2O_6$+$Mg_2Si_2O_6$+$Fe_2Si_2O_6$)), etc. These values are distinct from the values Ca/(Ca+Mg+Fe), and Mg/(Ca+Mg+Fe), and Fe/(Ca+Mg+Fe), which are included among the atomic ratios printed previously (Figure 2B). The atomic-ratio calculations use the abundance of each cation; the Wo-En-Fs calculation uses abundances of the three components. Because during the norm calculation, some Ca, Mg, and Fe are likely to be assigned to other components before Wo, En, and Fs are calculated, the two sets of calculations are not likely to yield similar values. The difference will be particularly noticeable for aluminous augite, because calcium is removed as $CaAlSiAlO_6$ before the component $Ca_2Si_2O_6$ (Wo) is calculated.

PROGRAMMER INFORMATION

This section is primarily intended for those who would like to pursue details within the program, or modify it. MINCLC consists of a short main program with 15 subroutines and a block data segment (BLKDAT). Listings of code are included as Appendices I and II. Figure 4 is a schematic chart of the operation of the main sequence of the MINCLC program. The main direction of flow in the program is downward. Some subroutines (CHECK, ITYPEn,

ICPLUS) that are only accessed through another subroutine are shown on the side in figure 4. ICPLUS is only called if the element list needs to be expanded from the original input list. The program ends by reaching an end-of-file marker when it attempts to read and decode in subroutines READER and CHECK.

The program handles one analysis at a time. It performs all applicable calculations, prints the results, resets arrays, and then looks for the next title line, control line, or an end of file.

SUBROUTINES

A brief description of each of the major subroutines in the program follows. Unless otherwise stated, the subroutines are called from the MAIN program.

TABLE 2: prints on the header page the current set of element names, valences, atomic weights, oxygen equivalents, and array position.

READER: reads the data from the input file.

CHECK: examines each line from the input file to determine whether it is a title, data, or control line. CHECK is called from the READER subroutine and uses the decode command to determine what it is reading.

NORMAL: prepares a normalized list of atomic fractions and prints it.

RATIOS: calculates and prints various cation ratios of interest.

SITEOC: uses normalized cation fractions to calculate a formal set of site occupancies for a pyroxene. (This subroutine is skipped if cations are not equal to 4.)

PXNORM: calculates a pyroxene norm by associating the ions in each site as molecules or components. This subroutine is skipped if the cations are not equal to 4, the anions are not equal to 6, or the weight percent value of SiO_2 is not greater than 20. A set of 64 components is actually used, and the order is determined by a data statement (norder) in BLKDAT. Each of the four individual sites in the pyroxene is set up from arrays in BLKDAT. Only those components that are used are printed out. Residuals of elements that were not completely used during the component calculation are printed at the end.

ITYPEn (n=1,2,3,4,5): are called from PXNORM and all function in the same manner. The subroutine calculates the amount of a particular component by filling its sites from the cation array. The amount of a particular component is determined by the smallest amount of one of the cations present in the component, and the cation amounts used for the component are then subtracted from the appropriate cation-array elements. The type for each component is set up in the itype array in BLKDAT. [note: Actually 6 types of pyroxene components are considered (see

table 4), but type 1 pyroxenes are always calculated in PXNORM for Ca, Mg, Fe. In the PXNORM subroutine, the similarity of pyroxene types is shown when the itype subroutines are called. For example: the type 2 subroutine may be called three times, each with a different arrangement for the sites. In this way the number of pyroxene component types is reduced to six.]

REDOX: is used only if it is called and only if the difference between the calculated anion total and the ideal anion total is greater than 0.0005. First, the routine adjusts the amount of silica in the analysis to achieve a desired anion:cation ratio and prints a warning message. Then the adjustment is repeated, using variable oxidation state elements to eliminate the discrepancy. As soon as the difference is corrected, the calculation is assumed to be complete. The cation amount of both the reduced and oxidized state of the element are changed (without making one negative) and then weight-percent amounts for each are recalculated. The values are only printed out when the program goes to the NORMAL subroutine (using a flag to indicate that REDOX has been used).

ICPLUS: a subroutine called from REDOX which expands the list of element names being used if only one valence state of an element was used in the input list.

RESET: a subroutine to reset counters and array elements to their starting values before a new data entry is read.

VARIABLES AND ARRAYS

Many variables are used in this program to maintain versatility and to facilitate changes to the program. A list is given below, in alphabetical order, of some of the variables and arrays used in MINCLC. A short accompanying explanation clarifies the ways in which each variable or array is used in the program. Most of the arrays described are used in several subroutines. To eliminate confusion caused by the similarity of the array names, a few local arrays are also described.

anions: number of anions used for calculating the mineral formula. This variable is customarily set by the user when the IONS option is specified (**** record); BLKDAT assigns it a default value of 6.0 if no value has been specified.

catfra, catrfc, cat: three arrays associated with the cation proportions of the analysis. Catfra is the cation fraction relative to the specified number of anions (default = 6.0). Catfrc is the fraction relative to the specified number of cations (default = 4.0). The cat array is constructed from the catfrc array, but the entries in the two arrays are in a different order. The cat array entries are ordered by atomic number, and the catfrc entries are ordered by input list order. For example: catfrc(6) and cat(14) would both contain the cation fraction for Si if Si is the 6th entry in the input list. [See subroutine NORMAL, do 700 loop.]

cation: number of cations used for calculating the mineral formula, set in the same way as anions. The default value from BLKDAT is 4.0.

ELNAM and elname: element name lists, the two arrays are identical except that in ELNAM, the element names are all capital letters (FE) and are recognized as input, and in elname, they are mixed (Fe) and are used in printing output.

eluse: an array used only in CHECK and READER to read in the elements from the input list. The element names are matched with names listed in the ELNAM array, and the code (element name) is then stored in the elused array.

elused: array constructed in READER, which contains the names of the elements in use for the current analysis.

err: a variable that acts as a lower limit in several calculations. It is set in BLKDAT (0.0001), but it is used in the program as er5 (0.0005 = 5*err). This "error" limit is used in the REDOX and PXNORM subroutines to determine whether a calculation is complete.

ib: the number of entries allowed on an input card, used only in READER.

ic: a counter for the number of elements being used for an analysis. (The value of ic is increased if needed when a redox calculation is made by calling the ICPLUS subroutine.)

id: a marker for the maximum number of elements being used (set equal to 30 in BLKDAT).

idcode(x): an array containing the position of element x in the input list.

idct: a "place holder" that acts as a marker between the original number of elements used in the input and any added elements from ICPLUS. This variable is used so that elements added in icplus will not be printed if they are equal to 0.

idont(y): a flag array that is set in CHECK to flag the options selected on a control card. It is used in conjunction with the subs(n) array. If idont(y) = 1, the option was not selected.

isite(n),n=1,2,3,4 and itype: arrays that are set in BLKDAT and used in the ITYPEn subroutines to generate pyroxene components. These five arrays are used together as shown below:

array position	isite1	isite2	isite3	isite4	itype
1	19 (K)	12 (Mg)	22 (Ti)	14 (Si)	4
2	19 (K)	28 (Ni)	22 (Ti)	14 (Si)	4
3	19 (K)	26 (Fe)	22 (Ti)	14 (Si)	4
4	19 (K)	33 (C2)	22 (Ti)	14 (Si)	4
.	.	.	.	.	.
.	.	.	.	.	.

The isite arrays contain the element codes (element name shown for

reference) for each of the four pyroxene sites that correspond to the type pyroxene indicated in the itype array. The norder array (see below) determines the order in which these components are used.

IZ: the array position of the last element name recognized by the program and set in BLKDAT. The element name for IZ in the ELNAM and elname arrays is $$, which is used as a marker for the end of the input element list.

i40: the maximum size of the internal arrays (ELNAM, elname, ianion, etc.) which contain all elements recognized by the program. The value for i40 is specified in BLKDAT and is used in the program as a loop terminator, when variables are being reset. The value of i40 cannot exceed the value of the array dimension declarators in the main program segment.

JSHn (n=1,2,3,4,5,8): flags that signal jumps (for use with DEC Fortran IV on the PDP 11/23).

JSH1 -- indicates an unsuccessful redox calculation attempt.

JSH2,3,4 -- used internally in the PXNORM subroutine to indicate the types of pyroxenes in the calculation.

JSH5 -- indicates that a redox calculation was done.

JSH8 -- flag used so that the table at the beginning of the output is only printed once.

ncode(z): an array containing the position of element Z from the input list in the program's internal arrays.

ncomp: the number of components used for pyroxene norm calculation; it is set (=64) in BLKDAT, but it can be changed if the ORDR option is used on a control record.

norder: an array listing the order in which the elements in the isiten arrays are used to make pyroxene components. For example: norder= (1,3,5,7,9...) so the first, third, and fifth elements in the isite and itype arrays are used to calculate the first, second, and third pyroxene components. Norder is set by a data statement in BLKDAT, but it can be changed by using the ORDR option on the control record and a record following it specifying the order desired.

numat: an array of the atomic numbers for each element recognized by the program, listed in the order in which the elements are stored in the programs's internal arrays.

subs(n): an alphabetic array of the possible entries for control record options, used to identify the options chosen. The options are signaled by setting the appropriate flag in the idont array (in the CHECK subroutine). The names recognized are: **** (used to identify that a control line has been read), RDOX, IONS, and ORDR. These names are read,

and if they have been flagged in subroutine CHECK, the options are performed at the appropriate place in the program. There are default conditions for IONS (4 cations, 6 anions) and ORDR (64 components, the norder array which is filled in BLKDAT).

title: an array containing the analysis title (as many as 72 characters).

wtper: an array of the oxide weight percent values for the current analysis.

wtpr: an array into which the weight percent oxides are read from the input list (in CHECK). This array is used in READER to fill the wtper array.

IDENTIFYING AN ELEMENT NAME WITHIN THE PROGRAM

One of the primary features of MINCLC's flexibility is that a large number of elements can be recognized by the program, and the elements can be varied or listed in an order that changes from one analysis to the next. The cost of this flexibility is that arrays must be used to identify both the position of the element in the input list (idcode) and the position of the element in the program's internal list of elements (ncode). The necessary arrays are constructed, and the matches between these arrays are tested in subroutine READER. For an input record consisting of:

SI 41.45AL 23.50FE 10.77MG 18.80CA 5.09MN 0033TI 0051

the first 3 entries of the various arrays would be set as shown below.

The analysis is first read in subroutine CHECK, where the eluse and wtpr arrays are only used to hold the data exactly as it is listed in the input record. The arrays are set up as follows:

eluse(1) = SI wtpr(1) = 41.45

eluse(2) = AL wtpr(2) = 23.50

eluse(3) = FE wtpr(3) = 10.77

The eluse and wtpr arrays set up in subroutine CHECK are then passed back to subroutine READER, where the information they contain is identified and stored in the arrays that are used throughout the program. The contents of the eluse array are compared with the possible elements listed in ELNAM, and if a match is obtained, the following arrays are constructed:

eluse(1) = ELNAM(14) elused(1) = elname(14) wtper(1) = wtpr(1)

eluse(2) = ELNAM(13) elused(2) = elname(13) wtper(2) = wtpr(2)

eluse(3) = ELNAM(26) elused(3) = elname(26) wtper(3) = wtpr(3)

ncode (1, 2, 3) = 14, 13, 26 idcode (14, 13, 26) = 1, 2, 3

catfrc(1) = wtpr(1)/atwtox(14)

catfrc(2) = wtpr(2)/atwtox(13)

```
catfrc(3) = wtper(3)/atwtox(26)
```

In the subroutine NORMAL, various cation arrays are set up for each of the elements as follows:

```
catfra(1) = catfrc(1) * total

catfrc(1) = catfrc(1) * total

cat(14) = catfrc (1)
```

The catfrc and cat arrays are then used in the calculations for several subroutines (REDOX, RATIOS, SITEOC, AND PXNORM).

INSTRUCTIONS FOR ALTERING THE PYROXENE NORM CALCULATION

The number of components and the order in which pyroxene norm components are calculated can be changed by calling for the ORDR option on the ****control line. Knowledge of FORTRAN is not necessary to use the option, but several data arrays in the program contain information needed to change the order of calculation, as explained below. First, when ORDR is specified on the **** control line, the total number of components that will be used is entered in columns 71-80 of the same line (integer value; right-justified). Three extra lines then follow the ****control record, listing the desired order for calculation of the components. Blank lines should be used if the number of components does not require all 3 lines. The pyroxene components are stored in the isiten arrays, and the order in which the components are used is stored in the norder array. The lines that follow the ****control line consist of integers (40I2 format), which list the next entries to use from the isiten and itype arrays. These lines form a new norder array.

Appendices III and IV are both lists of the array contents, which, when combined, make up the pyroxene norm components that can be calculated. Appendix III shows the components in the default order of calculation. Appendix IV is a list of the contents of the isiten arrays in the order in which they are stored. The itype array is also included in the list for reference. The entries in the table for the isiten arrays consist of the code used in the array for that element and its corresponding element name. To construct a new order for component calculation, use the array position numbers (Appendix IV) in the desired order on the lines following the ****ORDR line. For example: a list for the order of component calculation might begin with the entries: 1, 3, 5, 7, 9, 11, 13, 17, 19, 14, ...n until the desired number of components has been listed. (This is actually the default order used in the program, and the components are shown in that order in Appendix III.) No commas are used between the array position numbers, and if a blank is encountered before all the desired components have been read, an error message will be printed. An error message is also printed if less than 3 lines are used for the components list. (If either of the above errors is encountered, the norm is still calculated and the program continues, but the titles for the analyses that follow may be misread or skipped.)

The ORDR option merely allows for a change in the order of calculation of the recognized pyroxene components. If new components are needed to

accommodate significant amounts of an element that has not been included in the components used here (i.e. phosphorus, Goodrich, 1983), then major program changes are required. These changes would involve assigning cations to sites (isiten arrays), recognizing a "type" for the pyroxene (itype array), and determining where in the hierarchy (norder array) the component should be included.

INCREASING THE NUMBER OF ELEMENTS RECOGNIZED BY THE PROGRAM

MINCLC has been set up so that adding more elements is fairly straight forward, because most of the changes can be made in the BLKDAT section. The arrays that need to have additions made are: anion, ianion, ELNAM, elname, atwtox, and numat. The easiest way to add elements is to put them on the end of each of these arrays. Some code may need to be changed in the program if the positions of some existing elements in the arrays change (i.e., RATIOS, REDOX, SITEOC, PXNORM, and TYPE5 all contain some arrays or array numbers that use the ncode positions in calculations). Two other requirements must be followed: First, the value for IZ must be changed, and "$$" must move in the element name lists to the position following the last element name that the program recognizes. The second requirement is that the last entry in the ELNAM and elname arrays be a blank, because it is used to help check for data-entry errors. If the arrays must be expanded, the value of i40 must also be changed (in BLKDAT) to match the size of the arrays, and larger arrays must be declared in the main program segment and the subroutines.

If the program is to print different or more ratios, the only changes necessary are in the RATIOS subroutine. Other elements can be added with the appropriate ratio calculation and printing sections added, because the first section of the ratios subroutine defines names used only locally.

Acknowledgements

During the period in which the original program Mincalc was written, Freeborn was supported by the National Aeronautics and Space Administration (NASA) Contract T-2356-A to the USGS (J .S. Huebner, principal investigator). Huebner was partially supported through NASA Contract T-781-H while he converted Mincalc to MINCLC and participated in the preparation of this report. Malcolm Ross of the USGS kindly provided the previously unpublished list of normative pyroxene components and the default sequence in which they are calculated.

References

Cross, W., Iddings, J. P., Pirsson, L. V., and Washington, H. S. (1903) Quantitative classification of igneous rocks. Chicago: University of Chicago Press. 286 pages.

Goodrich, C. A. (1983) Phosphorus pyroxene and olivine in silicate inclusions in natural iron-carbon alloy from Uivfaq, Disko Island, Greenland. EOS, Transactions American Geophysical Union, v. 64, n. 45, p. 903.

References (continued)

Huebner, J. S. (1983) RDARL4, a FORTRAN interface for transferring chemical analytical data from an Applied Research Laboratories electron microprobe to a PDP-11 computing system. U.S. Geological Survey Open File Report 83-713, 40 pages.

Ikeda, Ko (1979) Calculating procedure of end-members of clinopyroxene, computer program and estimation of ferric and ferrous in EPMA analyses. Journal of the Japanese Association of Mineralogists, Petrologists, and Economic Geologists, v. 74, n. 4, p. 135-149.

Petersen, Erich U., Anovitz, Lawrence M., and Essene Eric J. (1984) Donpeacorite, (Mn, Mg)$MgSi_2O_6$, a new orthopyroxene and its proposed phase relations in the system $MnSiO_3$-$MgSiO_3$-$FeSiO_3$. American Mineralogist, V. 69, n. 4-5, p. 472-480.

Robinson, Peter (1980) The composition space of terrestrial pyroxenes - internal and external limits. In C. T. Prewitt, Ed., Reviews in Mineralogy, Vol. 7, Pyroxenes, p. 419-494. Mineralogical Society of America, Washington, D. C.

Smyth, J. R., (1980) Cation vacancies and the crystal chemistry of breakdown reaction in kimberlite omphacites. American Mineralogist, v. 65, n. 11-12, p. 1185-1191.

Table 1. Control arguments for MINCLC, used in a control record to instruct the program about the options to be used.

RDOX: the oxidation/reduction calculation is to be used as needed.

IONS: new anion and cation totals are to be used; the actual values (F10.0) desired are put in columns 51-60 and 61-70 of this line.

ORDR: a new order of calculation of normative components is to be used. The number of components desired is put in columns 71-80. (This control argument will require another line in the input file; see "Pyroxene Norm" section and instructions for altering the pyroxene norm calculation.) This option will only have an effect if the cation:anion ratio is 4:6.

Table 2. Chemical symbols, valence, form of input, and oxygen equivalents

Atomic Number	Symbol	Array Position	Valence	Input Component	Calculated Ion Charge		Oxygen Equivalent
1	H	1	+1	H_2O	OH	-1	-0.5
2	He	2	0	He	He	0	0.0
3	Li	3	+1	Li_2O	Li	+1	0.5
4	Be	4	+2	BeO	Be	+2	1.0
5	B	5	+3	B_2O_3	B	+3	1.5
6	C	6	+4	CO_2	C	+4	2.0
7	N	7	+5	N_2O_5	N	+5	2.5
8	O	8	-2	O	O	-2	-1.0
9	F	9	-1	F	F	-1	-0.5
10	Ne	10	0	Ne	Ne	0	0.0
11	Na	11	+1	Na_2O	Na	+1	0.5
12	Mg	12	+2	MgO	Mg	+2	1.0
13	Al	13	+3	Al_2O_3	Al	+3	1.5
14	Si	14	+4	SiO_2	Si	+4	2.0
15	P	15	+5	P_2O_5	P	+5	2.5
16	S1	35	-1	S	S	-1	-0.5
16	S2	36	-2	S	S	-2	-1.0
16	S6	16	+6	SO_3	S	+6	3.0
17	Cl	17	-1	Cl	Cl	-1	-0.5
18	Ar	18	0	Ar	Ar	0	0.0
19	K	19	+1	K_2O	K	+1	0.5
20	Ca	20	+2	CaO	Ca	+2	1.0
21	Sc	21	+3	Sc_2O_3	Sc	+3	1.5
22	Ti	22	+4	TiO_2	Ti	+4	2.0
22	Ts	32	+3	Ti_2O_3	Ti	+3	1.5
23	V	23	+5	V_2O_5	V	+5	2.5
24	Cr	24	+3	Cr_2O_3	Cr	+3	1.5
24	C2	33	+2	CrO	Cr	+2	1.0
25	Mn	25	+2	MnO	Mn	+2	1.0
25	Mc	34	+3	Mn_2O_3	Mn	+3	1.5
26	Fe	26	+2	FeO	Fe	+2	1.0
26	Fc	31	+3	Fe_2O_3	Fe	+3	1.5
27	Co	27	+2	CoO	Co	+2	1.0
28	Ni	28	+2	NiO	Ni	+2	1.0

Table 2. Chemical symbols, valence, form of input, and oxygen equivalents--Con't.

Atomic Number	Symbol	Array Position	Valence	Input Component	Calculated Ion Charge		Oxygen Equivalent
29	Cu	29	+1	Cu_2O	Cu	+1	0.5
30	Zn	30	+2	ZnO	Zn	+2	1.0
31	Ga	68	+3	Ga_2O_3	Ga	+3	1.5
33	As	37	-2	As	As	-2	-1.0
34	Se	38	-2	Se	Se	-2	-1.0
37	Rb	39	+1	Rb_2O	Rb	+1	0.5
38	Sr	40	+2	SrO	Sr	+2	1.0
39	Y	41	+3	Y_2O_3	Y	+3	1.5
40	Zr	42	+4	ZrO_2	Zr	+4	2.0
41	Nb	43	+5	Nb_2O_5	Nb	+5	2.5
42	Mo	44	+6	MoO_3	Mo	+6	3.0
46	Pd	45	+2	PdO	Pd	+2	1.0
47	Ag	46	+1	Ag_2O	Ag	+1	0.5
4B	Cd	47	+2	CdO	Cd	+2	1.0
50	Sn	48	+4	SnO_2	Sn	+4	2.0
51	Sb	49	+5	Sb_2O_5	Sb	+5	2.5
52	Te	50	-2	Te	Te	-2	-1.0
55	Cs	51	+1	Cs_2O	Cs	+1	0.5
56	Ba	52	+2	BaO	Ba	+2	1.0
57	La	67	+3	La_2O_3	La	+3	1.5
58	Ce	53	+3	Ce_2O_3	Ce	+3	1.5
60	Nd	54	+3	Nd_2O_3	Nd	+3	1.5
62	Sm	55	+3	Sm_2O_3	Sm	+3	1.5
63	Eu	56	+3	Eu_2O_3	Eu	+3	1.5
72	Hf	57	+4	HfO_2	Hf	+4	2.0
73	Ta	58	+5	Ta_2O_5	Ta	+5	2.5
74	W	59	+6	WO_3	W	+6	3.0
78	Pt	60	+2	PtO	Pt	+2	1.0
79	Au	61	+1	Au_2O	Au	+1	0.5
80	Hg	62	+2	HgO	Hg	+2	1.0
82	Pb	63	+4	PbO_2	Pb	+4	2.0
83	Bi	64	+5	Bi_2O_5	Bi	+5	2.5
90	Th	65	+4	ThO_2	Th	+4	2.0
92	U	66	+4	UO_2	U	+4	2.0

Table 3. Pyroxene normative components which are calculated by the default mode

	M2 Site	M1 Site	T Sites
1	K	0.5 Mg + 0.5 Ti	2 Si
2	K	0.5 Fe + 0.5 Ti	2 Si
3	Li	0.5 Mg + 0.5 Ti	2 Si
4	Li	0.5 Fe + 0.5 Ti	2 Si
5	Na	0.5 Mg + 0.5 Ti	2 Si
6	Na	0.5 Fe + 0.5 Ti	2 Si
7	Ca	Ti	2 Al
8	Fe	Ti	2 Al
9	Mg	Ti	2 Al
10	Ca	Ti	2 Fc
11	Fe	Ti	2 Fc
12	Mg	Ti	2 Fc
13	Ca	Mg	Ti + Si
14	Ca	Fe	Ti + Si
15	Mg	Mg	Ti + Si
16	Fe	Fe	Ti + Si
17	K	Ts	2 Si
18	K	Cr	2 Si
19	K	Fc	2 Si
20	K	Al	2 Si
21	Li	Ts	2 Si
22	Li	Cr	2 Si
23	Li	Fc	2 Si
24	Li	Al	2 Si
25	Na	Ts	2 Si
26	Na	Cr	2 Si
27	Na	Fc	2 Si
28	Na	Al	2 Si
29	Ca	Ts	Al + Si
30	Ca	Cr	Al + Si
31	Ca	Fc	Al + Si
32	Ca	Al	Al + Si
33	Fe	Ts	Al + Si
34	Fe	Cr	Al + Si
35	Fe	Fc	Al + Si
36	Fe	Al	Al + Si
37	Mg	Ts	Al + Si
38	Mg	Cr	Al + Si
39	Mg	Fc	Al + Si
40	Mg	Al	Al + Si

Table 3. Pyroxene normative components which are calculated by the default mode--Con't.

	M2 Site	M1 Site	T Sites
41	Ca	Ts	Fc + Si
42	Ca	Cr	Fc + Al
43	Ca	Fc	Fc + Si
44	Fe	Ts	Fc + Si
45	Fe	Cr	Fc + Si
46	Fe	Fc	Fc + Si
47	Mg	Ts	Fc + Si
48	Mg	Cr	Fc + Si
49	Mg	Fc	Fc + Si
50	Ca	C2	2 Si
51	Fe	C2	2 Si
52	Mg	C2	2 Si
53	Ca	Ni	2 Si
54	Fe	Ni	2 Si
55	Mg	Ni	2 Si
56	Zn	Mg	2 Si
57	Zn	Fe	2 Si
58	Ca	Zn	2 Si
59	Mn	Mg	2 Si
60	Mn	Fe	2 Si
61	Ca	Mn	2 Si
62	Ca	Ca	2 Si
63	Fe	Fe	2 Si
64	Mg	Mg	2 Si

Table 4. Types of Pyroxene Components.

[No "type 5" used in the program. The elements listed in the Element Substitutions column are listed in the approximate order in which they are used. Types 2 and 3 have the more general forms: ABT_2O_6 and $ABCDO_6$, respectively.]

Type in Program	General Formula	Element Substitutions
Type 1	$R_2^{2+}Si_2O_6$	R^{2+}=Ca,Fe,Mg,(Mn,Zn)
Type 2	$R^{2+}TiR_2^{3+}O_6$	R^{2+}=Ca,Mn,Fe,Mg R^{3+}=Al, Fc
2	$R^{+}R^{3+}Si_2O_6$	R^{+}=K,Li,Na R^{3+}=Ts,Cr,Fc,Al
2	$R_a^{2+}R_b^{2+}Si_2O_6$	R_a^{2+}=Ca,Mn,Zn,Fe,Mg R_b^{2+}=Ni,Mg,Fe,C2,Mn,Zn
Type 3	$R_a^{2+}R_b^{2+}SiTiO_6$	R_a^{2+}=Ca,Mn,Fe R_b^{2+}=Mg,Fe,Mn
3	$R^{2+}R_a^{3+}SiR_b^{3+}O_6$	R^{2+}=Ca,Mn,Fe,Mg R_a^{3+}=Ts,Cr,Fe R_b^{3+}=Al,Fc
Type 4	$R^{+}R_{.5}^{2+}Ti_{.5}Si_2O_6$	R^{+}=K,Li,Na R^{2+}=Mg,Ni,Fe,C2
Type 6	$R^{2+}R_2^{3+}SiO_6$	R^{2+}=Ca,Mn,Fe,Mg R^{3+}=Al,Fc
Type 7	$R_2^{2+}SiTiO_6$	R^{2+}=Fe,Mg

Figure 1.

```
****RDOXIONS                                                    6.          4.
ACMITE CYP52,II CORE 5/14/82, ANALYST G. CZAMANSKE
SI  5290TI   838AL    32FE  2180MN     5MG   178CA   111NA  1260$$
****RDOXIONS                                                   24          14
METHUEN MUSCOVITE. Hydrous formula.
SI  4587AL  3869MG    10NA    64K   1008H    467$$
****RDOXIONS                                                 22.          14.
METHUEN MUSCOVITE. Analysis 1a,
SI  4587AL  3869MG    10NA    64K   1008$$
****RDOXIONS                                                  8.          5.
FSLA Lake County plagioclase
SI 51.42AL 30.76TI  0.04FC  0.24FE  0.17MG  0.05MN  0.00CA 13.42NA  3.52
K   0.23$$
FSLA Lake County plagioclase
SI 51.08AL 31.05TI  0.05FC  0.43FE  0.12MG  0.22MN  0.01CA 13.85NA  3.38
K   0.12LI 0.001BA 0.011SR 0.142$$
FSBO Benson Orthoclase
SI 63.42AL 19.24FC  0.11CR 0.001P   0.49PB 0.003SR  0.02BA  0.62MN 0.001
CA  0.08NA  0.36CU 0.002K  15.34B  0.010$$
```

Figure 1. Example of an input file. This file contains five analyses to be recalculated using four different formula units. First is a pyroxene to be recalculated to 6.0 anions and 4.0 cations; next is a dioctahedral mica (paragonite) to be recalculated to a hydrous (24.0 anions, 14.0 cations) and then an anhydrous (22.0 anions, 14.0 cations) formula unit; and the last three analyses are feldspars. The file contains three different kinds of records; each record has a distinctive format that can be recognized by the subroutine CHECK. The control record has format (A4,10A4,6X,2(F10.0),I10). The first four bytes must be ****; the control options are listed in Table 1. The title has format (18A4). Weight-percent data are entered in format (9(A2,F6.2),A2); data input is terminated by the appearance of $$ in an A2 field.

Figure 2A.

PROGRAM MINCALC WAS ORIGINALLY WRITTEN BY PHELPS FREEBORN IN 1977 FOR J S HUEBNER'S NASA-FUNDED PYROXENE PROJECT.

IT WAS MODIFIED FOR THE DEC PDP-11/23 BY HUEBNER, 01/25/82

THIS VERSION WAS COMPILED SEPTEMBER 8, 1983 AND IS CONFIGURED AS FOLLOWS:

ATOMIC NUMBER	ELEMENT SYMBOL	VALENCE	OXYGEN EQUIVALENT	ATOMIC WEIGHT	ARRAY POSITION	ATOMIC NUMBER	ELEMENT SYMBOL	VALENCE	OXYGEN EQUIVALENT	ATOMIC WEIGHT	ARRAY POSITION
1	OH	-1	-0.5	9.007	1	14	S1	-1	-0.5	32.064	35
2	He	0	0.0	4.003	2	16	S2	-2	-1.0	32.064	36
3	Li	1	0.5	14.938	3	33	As	-2	-1.0	74.922	37
4	Be	2	1.0	25.011	4	34	Se	-2	-1.0	78.960	38
5	B	3	1.5	34.809	5	37	Rb	1	0.5	93.470	39
6	C	4	2.0	44.009	6	38	Sr	2	1.0	103.619	40
7	N	5	2.5	14.007	7	39	Y	3	1.5	112.904	41
8	O	-2	-1.0	15.999	8	40	Zr	4	2.0	123.218	42
9	F	-1	-0.5	18.998	9	41	Nb	5	2.5	132.904	43
10	Ne	0	0.0	20.183	10	42	Mo	6	3.0	143.937	44
11	Na	1	0.5	30.990	11	46	Pd	2	1.0	122.399	45
12	Mg	2	1.0	40.311	12	47	Ag	1	0.5	115.870	46
13	Al	3	1.5	50.980	13	48	Cd	2	1.0	128.399	47
14	Si	4	2.0	60.084	14	50	Sn	4	2.0	150.688	48
15	P	5	2.5	70.971	15	51	Sb	5	2.5	161.748	49
16	S	6	3.0	80.061	16	52	Te	-2	-1.0	127.600	50
17	Cl	-1	-0.5	35.453	17	55	Cs	1	0.5	140.904	51
18	Ar	0	0.0	39.948	18	56	Ba	2	1.0	153.339	52
19	K	1	0.5	47.102	19	58	Ce	3	1.5	164.118	53
20	Ca	2	1.0	56.079	20	60	Nd	3	1.5	168.238	54
21	Sc	3	1.5	68.954	21	62	Sm	3	1.5	174.348	55
22	Ti	4	2.0	79.898	22	63	Eu	3	1.5	175.958	56
23	V	5	2.5	90.939	23	72	Hf	4	2.0	210.488	57
24	Cr	3	1.5	75.994	24	73	Ta	5	2.5	220.945	58
25	Mn	2	1.0	70.937	25	74	W	6	3.0	231.847	59
26	Fe	2	1.0	71.846	26	78	Pt	2	1.0	211.089	60
27	Co	2	1.0	74.932	27	79	Au	1	0.5	204.966	61
28	Ni	2	1.0	74.709	28	80	Hg	2	1.0	216.589	62
29	Cu	1	0.5	71.546	29	82	Pb	4	2.0	239.188	63
30	Zn	2	1.0	81.369	30	83	Bi	5	2.5	248.978	64
26	Fc	3	1.5	79.845	31	90	Th	4	2.0	264.036	65
22	Ts	3	1.5	71.898	32	92	U	4	2.0	270.028	66
24	C2	2	1.0	67.995	33	57	La	3	1.5	162.910	67
25	Mc	3	1.5	78.934	34	31	Ga	3	1.5	93.720	68
16	S1	-1	-0.5	32.064	35	0	**	0	0.0	0.000	69

New control arguments have been read
RDOXIONS 6. 4. 0

Figure 2A. The first page containing the optional table that shows the elements for which the program is configured. This table is printed by subroutine TABLE2 and reproduces all the constants contained in the block data program unit (Appendix II) that are necessary to recalculate a chemical analysis.

Figure 2B.

```
ACMITE CYP52,II CORE 5/14/82, ANALYST O. CZAMANSKE                                    12-OCT-83
The data were read as follows:
SI   52.90  TI    8.38  AL    0.32  FE   21.80  MN    0.05  MG    1.78  CA    1.11  NA   12.60  %%    0.00

ELEMENT VALENCE   WT %      IONS PER          IONS PER
                            6.0 ANIONS        4.0 CATIONS

   Si      4     52.9000      2.0705            1.9939
   Ti      4      8.3800      0.2466            0.2375
   Al      3      0.3200      0.0148            0.0142
   Fe      2     21.8000      0.7135            0.6872
   Mn      2      0.0500      0.0017            0.0016
   Mg      2      1.7800      0.1038            0.1000
   Ca      2      1.1100      0.0465            0.0448
   Na      1     12.6000      0.9561            0.9208

TOTALS           98.940       4.154             5.778
                           CATIONS PER       ANIONS PER
                           6.0 ANIONS        4.0 CATIONS


Al/(Al + Si) =  0.007
Ca/(Ca + Na) =  0.046
Fe2/(Fe2 + Mg) = 0.873          (Fe2 + Fe3)/(Fe2+Fe3 + Mg) =  0.873      Fe3/(Fe3 + Fe2) =  0.000
Fe2/(Fe2 + Mg + Mn) =  0.871    (Fe2 + Fe3)/(Fe2 + Fe3 + Mg+ Mn) =  0.871
Ca/(Ca + Fe + Mg) =  0.054      Fe/(Ca + Fe + Mg)=  0.826                Mg/(Ca + Fe + Mg) =  0.120
(Li + Na + K)/Al = 64.774       (Li + Na + K +2Ca)/Al = 71.080
Al/Ti =  0.598E-01               (Al + Fe3)/Ti =  0.598E-01

Formal site occupancies
Tetrahedral: 1.994 Si: 0.006 Al:
Eight-fold:  0.921 Na: 0.045 Ca: 0.002 Mn: 0.033 Fe:
Octahedral:  0.008 Al: 0.100 Mg: 0.238 Ti: 0.654 Fe:
SUM OF ANIONS IN FORMULA UNIT:  5.778

Normative composition of pyroxenes (version of 21 April 1977) written by P. Freeborn at the institution of M. Ross)
 20.000  Na (Mg Ti)0.5 Si2 O6
 27.505  Na (Fe Ti)0.5 Si2 O6
  1.422  Na Al Si2 O6
  0.160  Mn Fe Si2 O6
  2.241  Ca2 Si2 O6
 27.402  Fe2 Si2 O6

Wo  7.56    Fs 92.44    En  0.00

THE FOLLOWING ELEMENTS FAILED TO FIT THE ACCEPTED COMPONENTS
  0.432  Na
  0.419  Si
```

Figure 2B. First recalculation of a pyroxene showing the input data as actually read, lists of ions, cation ratios, formal site occupancy, and pyroxene norm.

Figure 2C.

```
ACMITE CYP52,II CORE 5/14/82, ANALYST G. CZAMANSKE                                    12-OCT-83
(CATION TO ANION RATIO ADJUSTED TO  4.01 6.0)
Addition of  0.444 moles of silicon ( 22.3 relative per cent) would balance the cation to anion ratio
This corresponds to a change of 11.77* weight per cent SiO2 and would make the total weight per cent 110.71
ACMITE CYP52,II CORE 5/14/82, ANALYST G. CZAMANSKE            (ADJUSTED)

ELEMENT VALENCE    WT %       IONS PER          IONS PER
                              6.0 ANIONS        4.0 CATIONS

   Si      4     52.9000       1.9939            1.9939
   Ti      4      8.3800       0.2375            0.2375
   Al      3      0.3200       0.0142            0.0142
   Fe      2      7.7233       0.2434            0.2434
   Mn      2      0.0500       0.0016            0.0016
   Mg      2      1.7800       0.1000            0.1000
   Ca      2      1.1100       0.0448            0.0448
   Na      1     12.6000       0.9208            0.9208
   Fe      3     15.6442       0.4437            0.4437

TOTALS           100.507       4.000             6.000
                               CATIONS PER       ANIONS PER
                               6.000 ANIONS      4.000 CATIONS


Al/(Al + Si) =  0.007
Ca/(Ca + Na) =  0.046
Fe2/(Fe2 + Mg) = 0.709          (Fe2 + Fe3)/(Fe2+Fe3 + Mg) =  0.873      Fe3/(Fe3 + Fe2) =  0.646
Fe2/(Fe2 + Mg + Mn) =  0.706    (Fe2 + Fe3)/(Fe2 + Fe3 + Mg+ Mn) =  0.871
Ca/(Ca + Fe + Mg) =  0.115      Fe/(Ca + Fe + Mg)=  0.627                Mg/(Ca + Fe + Mg) =  0.258
(Li + Na + K)/Al = 64.774       (Li + Na + K +2Ca)/Al = 71.080
Al/Ti =  0.598E-01               (Al + Fe3)/Ti =  1.93

Formal site occupancies
Tetrahedral: 1.994 Si: 0.006 Al:
Eight-fold:  0.921 Na: 0.045 Ca: 0.002 Mn: 0.033 Fe:
Octahedral:  0.008 Al: 0.100 Mg: 0.444 Fe: 0.238 Ti: 0.211 Fe:
SUM OF ANIONS IN FORMULA UNIT:  6.000

Normative composition of pyroxenes (version of 21 April 1977: written by P. Freeborn at the institution of M. Ross)
 20.000  Na (Mg Ti)0.5 Si2 O6
 27.505  Na (Fe Ti)0.5 Si2 O6
 44.372  Na Fe Si2 O6
  0.201  Na Al Si2 O6
  0.610  Ca Al Si Al O6
  0.160  Mn Fe Si2 O6
  1.936  Ca2 Si2 O6
  5.216  Fe2 Si2 O6

Wo 27.07    Fs 72.93    En  0.00

New control arguments have been read
REDOXIONS                                        24.       14.         0
```

Figure 2C. Analysis 2B after adjustment of the proportions of the multivalent elements by the REDOX subroutine.

Figure 2D.

METHUEN MUSCOVITE. Hydrous formula. 12-OCT-83
The data were read as follows:
SI 45.87 AL 38.69 MG 0.10 NA 0.64 K 10.08 H 4.67 ** 0.00 0.00 0.00

ELEMENT	VALENCE	WT %	IONS PER 24.0 ANIONS	IONS PER 14.0 CATIONS
SI	4	45.8700	6.0186	6.0745
AL	3	38.6900	5.9830	6.0386
MG	2	0.1000	0.0196	0.0197
NA	1	0.6400	0.1628	0.1643
K	1	10.0800	1.6871	1.7028
OH	-1	4.6700	4.0875	4.1255
TOTALS		100.050	13.871 CATIONS PER 24.0 ANIONS	24.223 ANIONS PER 14.0 CATIONS

Al/(Al + Si) = 0.499
Ca/(Ca + Na) = 0.000
Fe2/(Fe2 + Mg) = 0.000 (Fe2 + Fe3)/(Fe2+Fe3 + Mg) = 0.000
Ca/(Ca + Fe + Mg) = 0.000 Fe/(Ca + Fe + Mg)= 0.000 Mg/(Ca + Fe + Mg) = 1.000
(Li + Na + K)/Al = 0.309 (Li + Na + K +2Ca)/Al = 0.309

The cations were not normalized to 4. The site occupancy calculation has been skipped

The analysis was not normalized to 4 cations per 6 anions - the norm calculation has been skipped

Figure 2D. A recalculation of an analysis containing water. The example is a dioctahedral mica, muscovite; because no multivalent element is present, no change was made during redox adjustment and the second page is not shown.

Figure 3.

Algebraic example	"Real" example
(1) def = desired anions - calc. anions	(1) def = 6.00 - 5.778 = 0.222
(2) correction=2*def	(2) cor= 2(0.222)= 0.444
(3) [a]since def>0, cat(Fe)<cor	(3) 0.687 ≮0.444
(4a) cat(Fc) = cat(Fc)+cor	(4a) cat(Fc)= 0+0.444= 0.444
(4b) cat(Fe) = cat(Fe)-cor	(4b) cat(Fe)= 0.687-0.444= 0.243
(5a)[bc]wt.%(Fe)=cat(Fe)*at.wt.ox/totcat	(5a) wt.%(Fe)= (.243)(71.846)/2.265= 7.7
(5b) wt.%(Fc)=cat(Fc)*at.wt.ox/totcat	(5b) wt.%(Fc)= (.444)(79.846)/2.265= 15.65
(6) def=(2*def)-cor	(6) def = (.444)-(.444)=0

Notes:

Original FeO value = 21.80 wt% (Fe cation proportions = 0.687). Desired anions = 6.000, desired cations = 4.000, calculated anions before REDOX correction = 5.778.

a. If cat(Fe) < cor then cor = cat(Fe).

b. Totcat = desired cations/Σwt.%(i)/at.wt.ox(i).

   ie. totcat = 4/[(52.90/60.084) + (8.38/79.898) + (0.32/50.980) + ...]=2.265

c. These equations (step 5) are just the inverse of equations used to calculate cation functions (relative to the desired cation total) from the input oxide weight percents.

Figure 3. Mathematical steps for the adjustment of multivalent elements by the REDOX subroutine. The example is the pyroxene recalculated in Figure 2B and and 2C; detailed explanation is in the text.

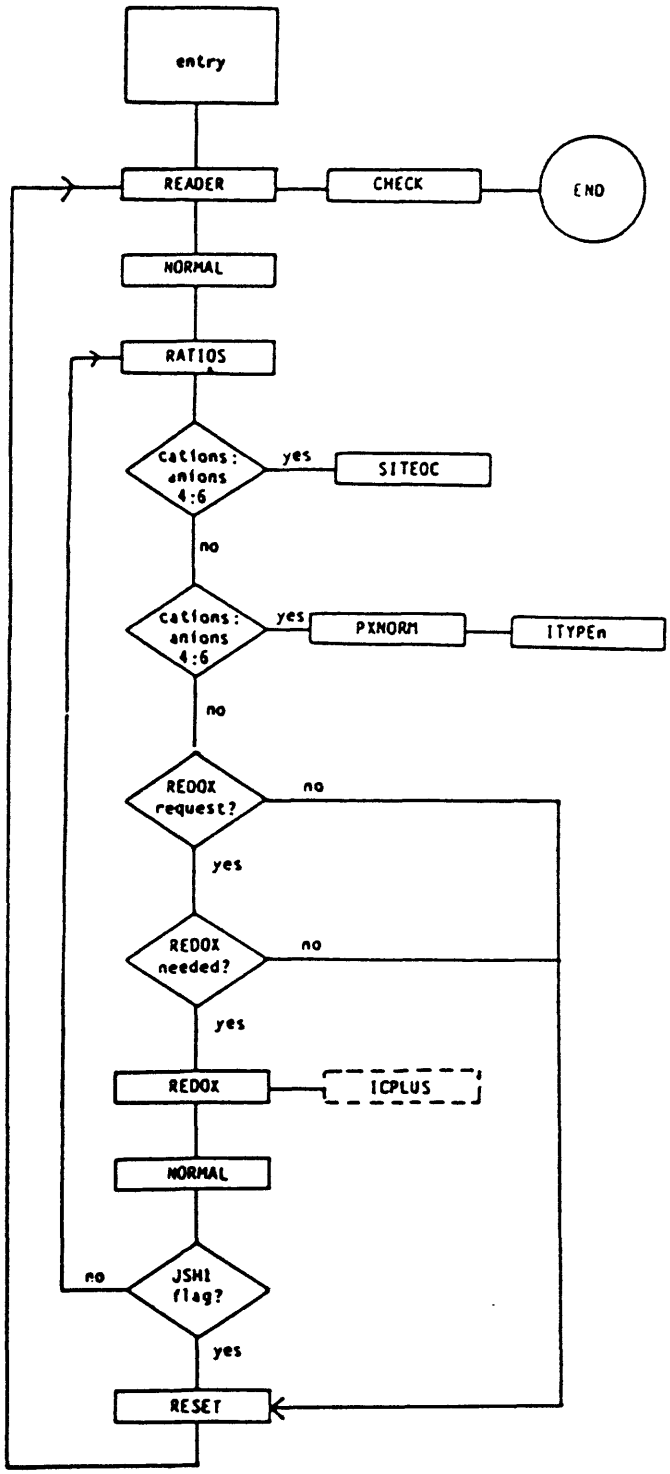

Figure 4. Schematic chart: Operation of the main segment of the MINCLC program

Appendix I. FORTRAN listing of the MINCLC program

```
      C PROGRAM MINCLC, ORIGINALLY WRITTEN BY PHELPS FREEBORN AS MINCALC,
C MODIFIED AND SIMPLIFIED BY J.S. HUEBNER FOR PDP-11 FORTRAN.
C MODIFICATIONS ARE INDICATED BY THE USE OF UPPER CASE CHARACTERS.
C THIS VERSION WAS COMPILED DECEMBER 14, 1983 AND LINKED TO BLKDAT
C
      DIMENSION woenfs(3),wtpr(30),elusd(30)
      BYTE REPLY,REPLY8
      COMMON/DATES/ADATE(5)
      COMMON/cats/catfra(30),catfrc(30),cat(70),anions,cation,
     &totcat,totan
      common/error/err
      common/flags/idont(4)
      common/names/elname(70),ELNAM(70)
      common/nos/ic,id,IZ,i40,ncomp,idct
      common/sites/isite1(99),isite2(99),isite3(99),isite4(99),
     &norder(99)
      common/titles/title(18),elused(30),wtper(30),
     &idcode(70),ncode(30),totwt
      common/types/itype(99)
      PRINT 300
300   FORMAT(1X,'PROGRAM MINCALC WAS ORIGINALLY WRITTEN BY PHELPS FREEBORN
     & IN 1977 FOR J S HUEBNER''S NASA-FUNDED PYROXENE PROJECT.',/)
      PRINT*,'IT WAS MODIFIED FOR THE DEC PDP-11/23 BY HUEBNER, 01/25/82'
      PRINT 400
400   FORMAT(1X,/,' THIS VERSION WAS COMPILED DECEMBER 14, 1983 AND IS
     & CONFIGURED AS FOLLOWS:',4(/))
      TYPE*,'THIS IS PROGRAM MINCLC, ORIGINALLY WRITTEN BY PHELPS FREEBORN'
      TYPE*,'AND MODIFIED FOR THE DEC MINC-23 BY J S HUEBNER.'
      TYPE*,'THIS VERSION OF MINCLC WAS COMPILED DECEMBER 14, 1983.'
      JSH8=1
      TYPE*,' '
      CALL DATE(ADATE)
      CALL IDATE(IDATE1,IDATE2,IDATE3)
      IF(IDATE1.NE.0) GOTO 460
      TYPE*,'Enter the date in any format, up to 20 characters:'
      ACCEPT 450,ADATE
450   FORMAT(5(A4))
460   TYPE*,' '
      TYPE*,'INCLUDE A TABLE OF ELEMENTS IN THE HEADER PRINTOUT? (Y or N)'
      ACCEPT 475,REPLY8
475   FORMAT(A1)
500   TYPE*,' '
      REPLY='N'
      TYPE*,'ENTER INPUT FILENAME AS DY?:??????.DAT'
      TYPE*,' '
      CALL ASSIGN(1,' ',-1)
      IF((JSH8.EQ.1).AND.(REPLY8.EQ.'Y')) CALL TABLE2
      er5=5.0*err
1000  call reader(REPLY)
      IF(REPLY.EQ.'Y') CLOSE(UNIT=1)
      IF(REPLY.EQ.'Y') GOTO 4000
      JSH5=1
2000  call normal(sumoxy,JSH5)
2020  call  ratios
      IF(CATION.EQ.4.) CALL SITEOC(SUMOXY)
      IF(CATION.EQ.4.AND.ANIONS.EQ.6.AND.WTPER(IDCODE(14)).GT.20.)
```

```
     & CALL PXNORM
C DETERMINE IF REDOX IS NECESSARY (REDOX MUST BE SPECIFIED ON **** LINE)
3400  defoxy=anions-sumoxy
      IF(ABS(defoxy)-er5) 4000,4000,3401
3401  IF(idont(2)-1) 3402,4000,3402
3402  CALL redox(defoxy,JSH1)
      JSH5=2
      CALL normal(sumoxy,JSH5)
      IF(JSH1.EQ.1)GO TO 4000  !JSH1=1 ONLY IF REDOX IS UNSUCCESSFUL
      go to 2020
4000  call reset
      IF(REPLY.EQ.'Y') GOTO 500
      GO TO 1000
      end
C
C --SUBROUTINE TABLE 2 PRINTS ON HEADER PAGE THE CURRENT SET OF ELEMENT NAM
C --VALENCES, ATOMIC WEIGHTS, OXYGEN EQUIVALENTS, AND ARRAY POSITIONS
C
      SUBROUTINE TABLE2(JSH8)
      COMMON/ATWTS/ATWTOX(70),NUMAT(70)
      COMMON/ANTS/ANION(70),IANION(70)
      COMMON/NAMES/ELNAME(70),ELNAM(70)
      COMMON/NOS/IC,ID,IZ,I40,NCOMP,IDCT
      PRINT 100
100   FORMAT(1X,'ATOMIC',6X,'ELEMENT',12X,'OXYGEN',4X,'ATOMIC',3X,'ARRAY',
     &11X,'ATOMIC',6X,'ELEMENT',12X,'OXYGEN',4X,'ATOMIC',3X,'ARRAY')
      PRINT 200
200   FORMAT(1X,'NUMBER',6X,'SYMBOL',2X,'VALENCE',2X,'EQUIVALENT',2X,
     &'WEIGHT',2X,'POSITION',9X,,'NUMBER',6X,'SYMBOL',2X,'VALENCE',2X,
     &'EQUIVALENT',2X,'WEIGHT',2X,'POSITION')
      M=IZ/2
      K=M+1
      IF(IZ.EQ.2*M) K=M
      DO 300, J=1,K
      PRINT 400,NUMAT(J),ELNAME(J),IANION(J),ANION(J),ATWTOX(J),J,
     &NUMAT(J+M),ELNAME(J+M),IANION(J+M),ANION(J+M),ATWTOX(J+M),J+M
300   CONTINUE
400   FORMAT(3X,I2,10X,A2,6X,I2,8X,F4.1,4X,F7.3,5X,I2,
     &14X,I2,10X,A2,6X,I2,8X,F4.1,4X,F7.3,5X,I2)
      JSH8=2
      RETURN
      END
C
C --SUBROUTINE READER READS DATA FROM INPUT FILE
C
      subroutine reader(REPLY)
      COMMON/ATWTS/atwtox(70),NUMAT(70)
      COMMON/DATES/ADATE(5)
      dimension wtpr(9),eluse(10)
      common/ants/anion(70),ianion(70)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,totan
      common/titles/title(18),elused(30),wtper(30),idcode(70),
     &ncode(30),totwt
      common/names/elname(70),ELNAM(70)
      common/nos/ic,id,IZ,i40,ncomp,idct
100   icheck=1
```

```
      call check(title,eluse,wtpr,icheck,REPLY)
      IF(REPLY.EQ.'Y') RETURN
      if(icheck.eq.2) goto 700   ! ICHECK=2 IF IT IS NOT A TITLE OR OPTION
110   PRINT 115,title,(ADATE(I),I=1,5)
115   format ('1',18a4,28X,5(A4),/,' The data were read as follows:')
      ib=9
      ic=0
      idct=0
      totcat=0.0
      totan=0.0
      icheck=2
200   call check(title,eluse,wtpr,icheck,REPLY)
      IF(REPLY.EQ.'Y') RETURN
      if(icheck.eq.1) goto 600
      PRINT 215,(eluse(i),wtpr(i),i=1,9)
215   format(1h ,9(a2,1x,f7.2,2x))
250   do 300 ja=1,10
      if(eluse(ja).eq.ELNAM(IZ)) goto 500
c     ELNAM(IZ)=$$ SIGNIFIES END OF DATA
      if(eluse(ja).eq.ELNAM(i40)) goto 300
c     ELNAM(I40)='BLANK'
c     search for element abbreviations in  list of element names
      do 400 jb=1,IZ
      if(eluse(ja).eq.ELNAM(jb)) goto 420
400   continue
      PRINT 405,eluse(ja),wtpr(ja)
405   format(1h0,'(',a2,2x,f6.2,') IS NOT AN ELEMENT NAME RECOGNIZED BY THIS
     & PROGRAM')
      goto 300
C     this routine rejects all except the first occurence of data for an
C    & element; IT INCREMENTS COUNTER AND CALCULATES CATIONS
420   if(idcode(jb).ne.id) goto 300
      ic=ic+1       !IC COUNTS HOW MANY ELEMENTS COME FROM INPUT LIST
      ncode(ic)=jb
      idcode(jb)=ic
      catfrc(ic)=wtpr(ja)/atwtox(jb)
320   if(ianion(jb)) 340,380,360
340   totan=totan+catfrc(ic)*(1.0+anion(jb))
      goto 380
360   totan=totan+catfrc(ic)*anion(jb)
      totcat=totcat+catfrc(ic)
380   wtper(ic)=wtpr(ja)
      elused(ic)=elname(jb)
300   continue
      if(ib.GE.id) goto 500
      ib=IB+9
      goto 200
c idct is a marker between original data and add-ons from redox
      idct=ic
500   if(ic.ne.0) return
      PRINT 505
505   format (1h0,'No data was accepted for this data set')
      goto 100
600   PRINT 605
605   format (1h0,'An error in the data records was found - a title
     & was read where data were expected',/,' that is there is
```

```
     &alphabetic information in positions 3 through 8 [format:
     &(8(a2,f6.2))]',/,' This analysis has been abandoned, see
     &next page\c.')
c     RESET has only a 'return' statement
      call reset
      GOTO 110
700   PRINT 215,(eluse(i),wtpr(i),i=1,9)
705   format (1h0,'An error is suspected on the following card',/,1h ,9(a2,
     &1x,f7.2,2x),2(2x,i4),/, ' (only numbers and blanks were found in
     &positions 3 through 8, an alphabetic character was expected)')
      go to 100
      end
C
C --SUBROUTINE CHECK IDENTIFIES THE KIND OF CARD JUST READ
C
      subroutine check(title,eluse,wtpr,icheck,REPLY)
      BYTE elem(80),numb(12)
      dimension card(20),eluse(10),wtpr(9),title(18),dont(10),subs(4)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      common/flags/idont(4)
      common/nos/ic,id,IZ,i40,ncomp,idct
      common/sites/isite1(99),isite2(99),isite3(99),isite4(99),
     &norder(99)
      data ndont,nsubs/4,4/
      data numb/' ','1','2','3','4','5','6','7','8','9','0','.'/
      data stars/'****'/
      data subs/'    ','RDOX','IONS','ORDR'/
10    READ(1,15,end=99,err=100) card
15    format (20a4)
      DECODE(80,25,card,err=70) elem
25    format(80a1)
      n=0
C  CHECK FOR NUMERAL OR BLANK
      do 20 i=3,8
      do 30 j=1,12
      if(elem(i).ne.numb(j)) goto 30
      n=n+1
      goto 20
30    continue
20    continue
      if(n.eq.6) goto 60
      icheck=1
      DECODE(80,45,card,err=50) title
45    format(18a4)
      if(title(1).eq.stars) goto 80
      GOTO 156
50    PRINT 55,card
55    format(1h0,'Error on following card, format used to read
     &was (18a4,2i4)',/,1h ,20a4)
      goto 10
C  READ INPUT ELEMENTS AND WEIGHT %'S HERE
60    DECODE(80,65,card,err=70) ((eluse(i),wtpr(i),i=1,9),ELUSE(10))
65    format(9(a2,f6.2),A2)
      icheck=2
      GOTO 156
```

```
70     PRINT 75,card
75     format (1h0,'Error on following card, format used to read
      &was (9(a2,f6.2),2i4)',/,1h ,20a4)
       icheck=1
       goto 10
C  READ OPTION CODES (**** LINE)
80     DECODE(80,85,card,err=90) dont,an,ct,nc
85     format(4x,10a4,6x,2f10.0,i10)
       PRINT 115,dont,an,ct,nc
115    format(/,' New control arguments have been read',/,1h
      &,10a4,10x,2f10.0,i10)
       do 110 i=1,ndont
110    idont(i)=1
       do 120 i=1,ndont
       do 130 j=1,nsubs
       if(dont(i).ne.subs(j)) goto 130
       idont(j)=0  !SET FLAG FOR MATCH OF OPTION, idont(j)=1 NO CHANGE
       goto 120
130    continue
120    continue
       if(idont(4).eq.1) goto 160
C CHANGE OF ORDER IN PXNORM REQUESTED
       ncomp=nc
       READ(1,145,err=150) norder
145    format(40i2)
       do 11 i=1,99
       if(norder(i).le.0) norder(i)=99
11     continue
160    if(idont(3).eq.1) goto 10
C  CHANGE IONS
       anions=an
       cation=ct
       goto 10
90     PRINT 95
95     format(1hl,'Error found while reading new control arguments
      &-program halted')
       stop
100    PRINT 105
105    format(1hl,'Error found while reading - subroutine check,
      &statement 10')
       stop
99     TYPE*,'Reached end of data - subroutine check, statement 10'
       TYPE*,' '
       TYPE*,'DO YOU WANT TO READ ANOTHER INPUT FILE? (Y or N)'
       ACCEPT 170, REPLY
170    FORMAT(A1)
       IF(REPLY.EQ.'Y') RETURN
       STOP 'GOOD BYE. HAVE A NICE DAY.'
150    TYPE*,'Error in data for new order for normative calculation'
156    RETURN
       end
C
C --SUBROUTINE RESET RESETS VARIABLES IN PREPARATION FOR NEXT ANALYSIS
C
       subroutine reset
       common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
```

```
     &totan
      COMMON/PATCH/MGERCT,NAERCT,MNERCT
      common/names/elname(70),ELNAM(70)
      common/nos/ic,id,IZ,i40,ncomp,idct
      common/titles/title(18),elused(30),wtper(30),
     &idcode(70),ncode(30),totwt
      do 100 i=1,i40
      cat(i)=0.0
      idcode(i)=id
100   continue
      do 200 l=1,id
      catfrc(l)=0.0
      catfra(l)=0.0
      wtper(l)=0.0
      ncode(l)=i40
      elused(l)=elname(70)
200   continue
      return
      end
C
C --SUBROUTINE NORMAL CALCULATES AND PRINTS ATOMIC FRACTIONS
C
      subroutine normal(sumoxy,JSH5)
      common/ants/anion(70),ianion(70)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,
     &totcat,totan
      common/names/elname(70),ELNAM(70)
      common/nos/ic,id,IZ,i40,ncomp,idct
      common/titles/title(18),elused(30),wtper(30),
     &idcode(70),ncode(30),totwt
      IF(JSH5.EQ.2) GOTO 550        !JSH5=2 MEANS REDOX ALREADY DONE
      totcat=cation/totcat
      totan=anions/totan
550   sumcat=0.0
      sumoxy=0.0
      totwt=0.0
c     CATERA IS NORMALIZED TO ANIONS; CATERC IS NORMALIZED TO CATION
c     SUMCAT IS THE NUMBER OF CATIONS PER ANIONS
c     SUMOXY IS THE NUMBER OF ANIONS PER CATION
      do 600 jc=1,ic
      nc=ncode(jc)
      catfra(jc)=catfrc(jc)*totan
      if(ianion(nc).le.0) goto 620
      sumcat=sumcat+catfra(jc)
620   catfrc(jc)=catfrc(jc)*totcat
640   if(ianion(nc)) 660,680,670
660   sumoxy=sumoxy+catfrc(jc)*(1.0+anion(nc))
      goto 680
670   sumoxy=sumoxy+catfrc(jc)*anion(nc)
680   totwt=totwt+wtper(jc)
600   continue
      PRINT 605
605   format (/,' ELEMENT VALENCE   WT %      IONS PER          IONS PER')
      PRINT 606,anions,cation
606   FORMAT(27X,F4.1,' ANIONS',7X,F4.1,' CATIONS',/)
      FACTOR=ANIONS/SUMOXY
```

```
      do 700 jd=1,ic
      nc=ncode(jd)
      if(nc.eq.IZ) goto 700
c section to skip printing of 0-value additions from redox
      if(JSH5.eq.1) goto 701
      if(jd.le.idct) goto 701
      if(wtper(jd).eq.0.00) goto 702
701   IF(JSH5.EQ.1) PRINT 705,elused(jd),ianion(nc),wtper(jd),
     &catfra(jd),catfrc(jd)
      IF(JSH5.EQ.2) PRINT 705,ELUSED(JD),IANION(NC),WTPER(JD),
     &FACTOR*CATFRA(JD),CATFRC(JD)
705   format(1h ,3x,a2,5x,i2,4x,f7.4,5x,f7.4,11X,F7.4)
702   cat(nc)=catfrc(jd)
700   continue
      IF(JSH5.EQ.2) GOTO 41
      PRINT 715,totwt,sumcat,sumoxy,anions,cation
715   format (/,' TOTALS',9x,f7.3,6x,f6.3,12X,F6.3,/,1h ,26x,'CATIONS PER',
     &7X,'ANIONS PER',/,1h ,25x,f4.1,' ANIONS',7X,f4.1,' CATIONS'/)
      return
 41   PRINT 716,totwt,FACTOR*sumcat,sumoxy,ANIONS,SUMCAT
716   FORMAT (/,' TOTALS',9X,F7.3,6X,F6.3,12X,F6.3,/,1H ,27X,'CATIONS PER',
     &7X,'ANIONS PER',/,1H ,26X,F6.3,' ANIONS',4X,F6.3,' CATIONS'/)
      RETURN
      end
C
C --SUBROUTINE RATIOS CALCULATES AND PRINTS ATOMIC RATIOS
C
      subroutine ratios
      REAL MG,MN,NA
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      alk=cat(3)+cat(11)+cat(19)
      Fe=cat(26)
      Fc=cat(31)
      Al=cat(13)
      Si=cat(14)
      Ti=cat(22)
      Mg=cat(12)
      Ca=cat(20)
      Na=cat(11)
      Mn=cat(25)
      fm=Fe+Mg
      fmn=Fe+Mg+Mn
      cfm=Ca+fm
      als=Al+Si
      can=Ca+Na
      PRINT 95
95    format(/)
      if(als.le.0.0) goto 100
      alsi=Al/als
      PRINT 105,alsi
105   format(' Al/(Al + Si) = ',f6.3)
100   if(can.le.0.0) goto 110
      cana=Ca/can
      PRINT 115,cana
115   format(' Ca/(Ca + Na) = ',f6.3)
```

```
110    if(fm.le.0.0) goto 120
       femg=Fe/fm
       fcmg=(Fe+Fc)/(fm+Fc)
       PRINT 125,femg,fcmg
125    format(' Fe2/(Fe2 + Mg) =',f6.3,'          (Fe2 + Fe3)/(Fe2
      &+Fe3 + Mg) = ',f6.3)
       if((Fe+Fc).le.0.0) goto 120
       fefc=Fc/(Fe+Fc)
       PRINT 127,fefc
127    format('+',72x,'Fe3/(Fe3 + Fe2) = ',f6.3)
120    if(Mn.le.0.0) goto 130
       femgn=Fe/fmn
       fcmgn=(Fe+Fc)/(fmn+Fc)
       PRINT 135,femgn,fcmgn
135    format(' Fe2/(Fe2 + Mg + Mn) = ',f6.3,'    (Fe2 + Fe3)/(Fe2
      &+ Fe3 + Mg+ Mn) = ',f6.3)
130    if(cfm.le.0.0) goto 140
       cafm=Ca/cfm
       cfem=Fe/cfm
       cfmg=1.0-cafm-cfem
       PRINT 145,cafm,cfem,cfmg
145    format(' Ca/(Ca + Fe + Mg) = ',f6.3,'      Fe/(Ca + Fe + Mg)
      &= ',f6.3,15x,'Mg/(Ca + Fe + Mg) = ',f6.3)
140    if(Al.le.0.0) goto 150
       alca=(alk+2.0*Ca)/Al
       alna=alk/Al
       if(alca.le.0.0) goto 150
       PRINT 155,alna,alca
155    format(' (Li + Na + K)/Al = ',f6.3,'       (Li + Na + K +
      &2Ca)/Al = ',f6.3)
150    if(Ti.le.0.001) goto 160
       if((Al+Fc).le.0.0) goto 160
       tial=Al/Ti
       tifa=(Al+Fc)/Ti
       PRINT 165,tial,tifa
165    format(' Al/Ti = ',g10.3,14x,'(Al + Fe3)/Ti = ',g10.3)
160    return
       end
C
C --SUBROUTINE SITEOC CALCULATES AND PRINTS A FORMAL PYROXENE SITE OCCUPANC
C --ONLY IF THE DESIRED ANIONS:CATION EQUAL 6:4
C
       subroutine siteoc(SUMOXY)
       REAL*4 nsite(3,3)
       dimension isite(12,3),jsite(3),xsite(3),cion(8),eion(30)
       common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
      &totan
       common/names/elname(70),ELNAM(70)
       common/nos/ic,id,IZ,i40,ncomp,idct
       common/titles/title(18),elused(30),wtper(30),idcode(70),
      &ncode(30),totwt
C  ISITE CONTAINS AT. #'S FOR ELEMENTS WHICH FIT THE THREE PYROXENE SITES
       data isite/14,13,31,22,8*0,
      &19,11,3,20,25,30,26,12,28,3*0,
      &13,12,31,28,22,24,32,33,34,26,25,30/
       data jsite/4,9,12/      !TOTAL SUM ALLOWED IN EACH SITE
```

```
      data nsite/'Tetr','ahed','ral:','Eigh','t-fo','ld: ',
     &'Octa','hedr','al: '/
      data xsite/2.0,1.0,1.0/
      PRINT 105
105   format (/,' Formal site occupancies')
C  FILL SITES IN ORDER: TETRA., EIGHTFLD, OCTAHEDR.
      do 200 i=1,3
      it=0
      site=xsite(i)
      do 300 j=1,jsite(i)
      ion=isite(j,i)
      if(cat(ion).le.0.0) goto 300
      it=it+1
      eion(it)=elname(ion)
      cion(it)=cat(ion)
      if(site.lt.cion(it)) cion(it)=site
      cat(ion)=cat(ion)-cion(it)
      site=site-cion(it)
      if(site.le.0.0) goto 220
300   continue
      if(it.eq.0) goto 800
220   PRINT 225,(nsite(j,i),j=1,3),(cion(j),eion(j),j=1,it)
225   format(1h ,3a4,12(f6.3,1x,a2,';'))
200   continue
      PRINT 250,SUMOXY
250   FORMAT(1H ,'SUM OF ANIONS IN FORMULA UNIT: ',F6.3)
      is=0
      sum=0.0
C  CHECK TO SEE IF IONS WERE ALL USED IN SITES
      do 500 i=1,ic
      ion=ncode(i)
      if(abs(cat(ion)).lt.0.001) goto 500
      is=is+1
      cion(is)=cat(ion)
      eion(is)=elname(ion)
500   continue
      if(is.eq.0) goto 600
520   PRINT 525,(cion(i),eion(i), i = 1,is)
525   format(' The following ions were not placed in a site',/,1h ,
     &18(f6.3,1x,a2,';'))
C  REFILL CAT ARRAY, NEEDED FOR NEXT CALCULATIONS
600   do 700 i=1,I40
      j=idcode(i)
      cat(i)=catfrc(j)
700   continue
      PRINT*,' '
      return
800   PRINT 805,(nsite(j,i),i=1,3)
805   format(1h0,'There were no cations to fill the ',3a4,' site')
      goto 600
      return
      end
C
C --SUBROUTINE PXNORM CALCULATES AND PRINTS NORMATIVE PYROXENE COMPONENTS
C --FOLLOWING THE SCHEME OF M. ROSS OF THE U.S. GEOLOGICAL SURVEY
C
```

```
      subroutine pxnorm (JSH2)
      dimension woenfs(3),wtpr(30),elusd(30)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      common/error/err
      common/names/elname(70),ELNAM(70)
      common/nos/ic,id,IZ,i40,ncomp,idct
      common/sites/isite1(99),isite2(99),isite3(99),isite4(99),
     &norder(99)
      common/types/itype(99)
      er5=5.0*err
80    do 90 i=1,3
      woenfs(i)=0.0
90    continue
      sum=0.0
      PRINT 8811
8811  FORMAT(' Normative composition of pyroxenes (version of 21 April
     &1977; written by P. Freeborn at the instigation of M. Ross)')
C  NORDER CONTAINS THE KEY ORDER FOR NORM CALCULATION
      do 100 j=1,ncomp
      i=norder(j)
      il=isite1(i)
      i2=isite2(i)
      i3=isite3(i)
      i4=isite4(i)
      ityp=itype(i)
C  COMPONENTS CALCULATED IN TYPEn SUBROUTINES,  JSHn ARE FLAGS FOR TYPES
      goto(1,2,3,4,6,7,8,9),ityp
1     call type1(il,i3,comp)
      JSH3=0
      GOTO 10
2     call type2(il,i2,i3,comp)
      JSH3=0
      GOTO 10
3     call type3(il,i2,i3,i4,comp)
      JSH3=0
      GOTO 10
4     call type4(il,i2,i3,i4,comp)
      JSH3=0
      GOTO 10
6     call type5(il,i2,i3,i4,comp)
      JSH3=0
      GOTO 10
7     call type2(il,i3,i2,comp)
      JSH3=6
      GOTO 10
8     call type2(i3,i4,il,comp)
      JSH3=7
      GOTO 10
10    JSH4=JSH2+JSH3
      GOTO(100,110,120,130,140,150,100,100,130,160),JSH4 !FOR PRINTING
9     PRINT 85,j,i
85    format('0INCORRECT TYPE CALLED',2(2x,i2))
      goto 100
C WO-EN-FS CALCULATED AFTER OTHER COMPONENTS
110   if(il.eq.20) k=1
```

```
      if(il.eq.26) k=2
      if(il.eq.12) k=3
      woenfs(k)=comp
      sum=sum+comp
      PRINT 115,comp,elname(il),elname(i3)
115   format(1h ,f7.3,1x,2(1x,a2,'2'),' 06')
      goto 100
120   PRINT 125,comp,elname(il),elname(i2),elname(i3)
125   format(1h ,f7.3,1x,3(1x,a2),'2 06')
      goto 100
130   PRINT 135,comp,elname(il),elname(i2),elname(i3),elname(i4)
135   format(1h ,f7.3,1x,4(1x,a2),' 06')
      goto 100
140   PRINT 145,comp,elname(il),elname(i2),elname(i3),elname(i4)
145   format(1h ,f7.3,2x,a2,' (',a2,1x,a2,')0.5 ',a2,'2 06')
      goto 100
150   PRINT 155,comp,elname(il),elname(i2),elname(22),elname(i3),
     &elname(i4)
155   format(1h ,f7.3,2x,a2,' (',a2,1x,a2,')0.5 ',a2,2x,a2,' 06')
160   PRINT 165,comp,elname(il),elname(i3),elname(i4)
165   format(1h ,f7.3,2x,a2,'2',2(1x,a2),' 06')
100   continue
      if(sum.le.0.0) goto 190
      do 180 i=1,3
      woenfs(i)=100.0*woenfs(i)/sum
180   continue
      PRINT 185,woenfs
185   format(/,' Wo',f6.2,'    Fs',f6.2,'    En',f6.2)
190   continue
3000  kk=0
C  CHECK FOR REMAINDERS NOT INCLUDED IN COMPONENTS
      do 3100 k=1,I40
      if(abs(cat(k)).le.er5) goto 3100
      kk=kk+1
      elusd(kk)=elname(k)
      wtpr(kk)=cat(k)
3100  continue
      if(kk.eq.0) return
      PRINT 3305
3305  format(/,' THE FOLLOWING ELEMENTS FAILED TO FIT THE
     &ACCEPTED COMPONENTS')
      do 3300 k=1,kk
      PRINT 3355,wtpr(k),elusd(k)
3355  format(1h ,f7.3,2x,a2)
3300  continue
      return
      end
C
C --SUBROUTINE REDOX ADJUSTS PROPORTIONS OF OXIDATION STATES OF MULTIVALENT
C --ELEMENTS, ATTEMPTING TO ACHIEVE THE DESIRED ANION:CATION RATIO. 8/15/83
C
      subroutine redox(def,JSH1)
      dimension iredox(8),atwtox(8)
      COMMON/DATES/ADATE(5)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
```

```
      common/error/err
      common/nos/ic,id,IZ,i40,ncomp,idct
      common/titles/title(18),elused(30),wtper(30),idcode(70),
     &ncode(30),totwt
C IREDOX SETS ORDER FOR TRYING VARIABLE OXIDATION ELEMENTS
      DATA IREDOX/ 32, 33, 26, 25, 22, 24, 31, 34 /
      DATA ATWTOX/ 71.898, 67.995, 71.846, 70.937, 79.898, 75.995,
     & 79.846, 78.937 /
C     INITIALIZE FLAG JSH1 THAT DETERMINES ACTION AFTER RETURN TO MAIN PROG
      JSH1=0
      PRINT 25,title,(ADATE(I),I=1,5),cation,anions
25    format (1h1,18a4,28X,5(A4),/1h ,'(CATION TO ANION RATIO ADJUSTED TO '
     &,f4.1,':',f4.1,')')
C ADJUSTING SI IN ANALYSIS--CAUTIONARY NOTE TO USER
      def=2.0*def                          !DEF=DEFOXY(main pgm)=ANIONS-SUMOX
      cor=def
      id14=idcode(14)
      if(catfrc(id14).le.0.0) goto 40
      corp=cor/catfrc(id14)
      corps=corp*wtper(id14)
      corpt=totwt+corps
      corp=100.0*corp
30    PRINT 35,cor,corp,corps,corpt
35    format (' Addition of ',f6.3,' moles of silicon (',
     &f5.1,' relative per cent) would balance the cation to anion
     &ratio',/,' This corresponds to a change of ',f5.2,'% weight per
     &cent SiO2 and would make the total weight per cent ',f6.2)
C  DECIDE WHETHER OXIDATION OR REDUCTION OF MULTIVALENT ELEMENTS NEEDED
40    IF(DEF) 110,200,50
C  SECTION FOR OXIDATIOIN
50    do 100 i=1,4
      j=i+4
      cor=def
      iro=iredox(J)
      ido=idcode(iro)
      if(ido.eq.id) call icplus(ic,ido,iro)
      irr=iredox(i)
      idr=idcode(irr)
      if(idr.eq.id) call icplus(ic,idr,irr)
140   if(catfrc(idr).lt.cor) cor=catfrc(idr)
160   catfrc(ido)=catfrc(ido)+cor
      catfrc(idr)=catfrc(idr)-cor
      wtper(idr)=catfrc(idr)*atwtox(i)/totcat
      wtper(ido)=catfrc(ido)*atwtox(j)/totcat
      def=def-cor
      if(abs(def).le.err) goto 200   !RATIO ACHIEVED. RETURN DIRECTLY
100   continue
      GOTO 101
C  SECTION FOR REDUCTION
110   DO 120, I=8,5,-1
      J=I-4
      COR=DEF
      IRO=IREDOX(I)
      IDO=IDCODE(IRO)
      IF(IDO.EQ.ID) CALL ICPLUS(IC,IDO,IRO)
      IRR=IREDOX(J)
```

```
      IDR=IDCODE(IRR)
      IF(IDR.EQ.ID) CALL ICPLUS(IC,IDR,IRR)
      IF(CATFRC(IDO).LT.-COR) COR=-CATFRC(IDO)
      CATFRC(IDO)=CATFRC(IDO)+COR
      CATFRC(IDR)=CATFRC(IDR)-COR
      WTPER(IDR)=CATFRC(IDR)*ATWTOX(J)/TOTCAT
      WTPER(IDO)=CATFRC(IDO)*ATWTOX(I)/TOTCAT
      DEF=DEF-COR
      IF(ABS(DEF).LE.ERR) GOTO 200
120   CONTINUE
101   def=-def/2.0
      PRINT 105,anions,def
105   format(1h0,'TOTAL OXYGENS - ',f6.3,' = ',f6.3,' AFTER
     &ADJUSTMENT OF ALL AVAILABLE MULTIVALENT ELEMENTS')
      sumoxy=anions-def
      totan=1.0
      totcat=1.0
C     FLAG JSH=1 PREVENTS MAIN FROM CALLING REDOX TWICE
190   JSH1=1
      Return
200   totan=1.0
      totcat=1.0
      PRINT 205,(title(i),i=1,15)
205   format(1H ,15a4, ' (ADJUSTED) ',i4,4x)
250   RETURN
      end
C
C --SUBROUTINE ICPLUS EXPANDS THE LIST OF ELEMENTS TO INCLUDE ADDITIONAL
C --REDOX STATES OF MULTIVALENT ELEMENTS
C
      subroutine icplus(ic,id,ir)
      common/names/elname(70),ELNAM(70)
      common/titles/title(18),elused(30),wtper(30),idcode(70),
     &ncode(30),totwt
      ic=ic+1
      ncode(ic)=ir
      elused(ic)=elname(ir)
      IDCODE(ir)=ic
      id=ic
      return
      end
C
C --SUBROUTINE TYPE 1 FOR PYROXENE COMPONENTS OF THE TYPE: R2(2+)SI2O6
C
      subroutine type1(ia,ib,comp,JSH2)
      dimension l(2)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      common/error/err
      l(1)=ia
      l(2)=ib
      dummy=cat(l(1))
      if(dummy.le.err) GOTO 300
      do 200 j=1,2
      cat(l(j))=cat(l(j))-dummy
200   continue
```

```
      comp=50.0*dummy
      JSH2=2
      return
300   JSH2=1
      RETURN
      end
C
C --SUBROUTINE TYPE 2 FOR PYROXENE COMPONENTS OF TYPE ABT2O6
C
      subroutine type2(ia,ib,ic,comp,JSH2)
      dimension l(3),factor(3)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      common/error/err
      data factor/2*1.0,2.0/
      l(1)=ia
      l(2)=ib
      l(3)=ic
      dummy=cat(l(1))
      do 100 i=2,3
      amt=cat(l(i))/factor(i)
      if(amt.lt.dummy) dummy=amt
100   continue
      if(dummy.le.err) GOTO 300
      do 200 j=1,3
      cat(l(j))=cat(l(j))-dummy*factor(j)
200   continue
      comp=100.0*dummy
      JSH2=3
      return
300   JSH2=1
      RETURN
      end
C
C --SUBROUTINE TYPE 3 FOR PYROXENE COMPONENTS OF TYPE ABCDO6
C
      subroutine type3(ia,ib,ic,id,comp,JSH2)
      dimension l(4)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      common/error/err
      l(1)=ia
      l(2)=ib
      l(3)=ic
      l(4)=id
      dummy=cat(l(1))
      do 100 i=2,4
      if(cat(l(i)).lt.dummy) dummy=cat(l(i))
100   continue
      if(dummy.le.err) GOTO 300
      do 200 j=1,4
      cat(l(j))=cat(l(j))-dummy
200   continue
      comp=100.0*dummy
      JSH2=4
      return
```

```
300   JSH2=1
      RETURN
      end
C
C --SUBROUTINE TYPE 4 FOR PYROXENES OF TYPE R(+)R.5(2+)TI.5SI2O6
C
      subroutine type4(ia,ib,ic,id,comp,JSH2)
      dimension l(4),factor(4)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      common/error/err
      data factor/1.0,2*0.5,2.0/
      l(1)=ia
      l(2)=ib
      l(3)=ic
      l(4)=id
      dummy=cat(l(1))
      do 100 i=2,4
      amt=cat(l(i))/factor(i)
      if(amt.lt.dummy) dummy=amt
100   continue
      if(dummy.le.err) GOTO 300
      do 200 j=1,4
      cat(l(j))=cat(l(j))-dummy*factor(j)
200   continue
      comp=100.0*dummy
      JSH2=5
      return
300   JSH2=1
      RETURN
      end
C
C --SUBROUTINE TYPE 5 FOR PYROXENE COMPONENTS OF TYPE R2(2+)SiTiO6
C
      subroutine type5(ia,ib,ic,id,comp,JSH2)
      dimension l(5),factor(5)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,
     &totan
      common/error/err
      data factor/1.0,0.5,1.0,1.0,0.5/
      l(1)=ia
      l(2)=ib
      l(3)=ic
      l(4)=id
      l(5)=22
      dummy=cat(l(1))
      do 100 i=2,5
      amt=cat(l(i))/factor(i)
      if(amt.lt.dummy) dummy=amt
100   continue
      if(dummy.le.err) GOTO 300
      do 200 j=1,5
      cat(l(j))=cat(l(j))-dummy*factor(j)
200   continue
      comp=100.0*dummy
      JSH2=6
      return
300   JSH2=1
      RETURN
      end
```

Appendix II. Block data program unit

```
C BLKDAT WAS ORIGINALLY WRITTEN BY PHELPS FREEBORN FOR PROGRAM MINCALC &
C MODIFIED BY J S HUEBNER WHEN MINCALC MODIFIED TO MINCLC FOR PDP-11/23
C
C SPECIFIES ELEMENT NAMES AND VALENCES (IN TERMS OF NUMBER OF OXYGENS
C NEEDED TO ACHIEVE CHARGE BALANCE), AND THE NATURE AND ORDER OF CALCULATION
C OF THE NORMATIVE PYROXENE COMPONENTS.
C
C LAST EDITED DECEMBER 12, 1983
C
      BLOCK DATA BLKDAT
      COMMON/ATWTS/ATWTOX(70),NUMAT(70)
      common/ants/anion(70),ianion(70)
      common/cats/catfra(30),catfrc(30),cat(70),anions,cation,totcat,totan
      common/error/err
      common/flags/idont(4)
      common/names/elname(70),ELNAM(70)
      common/nos/ic,id,IZ,i40,ncomp,idct
      common/sites/isite1(99),isite2(99),isite3(99),isite4(99),norder(99)
      common/titles/title(18),elused(30),wtper(30),
     &idcode(70),ncode(30),totwt
      common/types/itype(99)
C SPECIFY MAXIMUM NUMBERS OF ELEMENTS THAT CAN BE READ, RECOGNIZED, ETC.
      data id,IZ,i40/30,69,70/
      data ncomp/64/
C SET INITIAL OR DEFAULT VALUES
      data catfra,catfrc/60*0.0/
      data cat/70*0.0/
      data anions,cation/6.0,4.0/
      data err/0.0001/
      data idont/4*1/
C ANION ARRAY SPECIFIES NUMBER OF ANIONS ASSOCIATED WITH EACH ELEMENT
      data anion/
     &-0.5,  0.0,  0.5,  1.0,  1.5,  2.0,  2.5, -1.0, -0.5,  0.0,
     & 0.5,  1.0,  1.5,  2.0,  2.5,  3.0, -0.5,  0.0,  0.5,  1.0,
     & 1.5,  2.0,  2.5,  1.5,  1.0,  1.0,  1.0,  1.0,  0.5,  1.0,
     & 1.5,  1.5,  1.0,  1.5, -0.5, -1.0, -1.0, -1.0,  0.5,  1.0,
     & 1.5,  2.0,  2.5,  3.0,  1.0,  0.5,  1.0,  2.0,  2.5, -1.0,
     & 0.5,  1.0,  1.5,  1.5,  1.5,  1.5,  2.0,  2.5,  3.0,  1.0,
     & 0.5,  1.0,  2.0,  2.5,  2.0,  2.0,  1.5,  1.5,  2*0.0/
C IANION ARRAY CONTAINS VALENCES OF THE ELEMENTS IN ELEMENT NAME ARRAYS
      data ianion/
     &-1, 0, 1, 2, 3, 4, 5,-2,-1, 0,
     & 1, 2, 3, 4, 5, 6,-1, 0, 1, 2,
     & 3, 4, 5, 3, 2, 2, 2, 2, 1, 2,
     & 3, 3, 2, 3,-1,-2,-2,-2, 1, 2,
     & 3, 4, 5, 6, 2, 1, 2, 4, 5,-2,
     & 1, 2, 3, 3, 3, 3, 4, 5, 6, 2,
     & 1, 2, 4, 5, 4, 4, 3, 3, 2*0/
C ELNAM ARRAY CONTAINS ELEMENT SYMBOLS RECOGNIZED AS INPUT
      data ELNAM/
     &'H ','HE','LI','BE','B ','C ','N ','O ','F ','NE',
     &'NA','MG','AL','SI','P ','S6','CL','AR','K ','CA',
     &'SC','TI','V ','CR','MN','FE','CO','NI','CU','ZN',
     &'FC','TS','C2','MC','S1','S2','AS','SE','RB','SR',
     &'Y ','ZR','NB','MO','PD','AG','CD','SN','SB','TE',
     &'CS','BA','CE','ND','SM','EU','HF','TA','W ','PT',
```

```
     &'AU','HG','PB','BI','TH','U ','LA','GA','$$','  '/
C ELNAME ARRAY CONTAINS ELEMENT SYMBOLS PRINTED OUT
      data elname/
     &'OH','He','Li','Be','B ','C ','N ','O ','F ','Ne',
     &'Na','Mg','Al','Si','P ','S6','Cl','Ar','K ','Ca',
     &'Sc','Ti','V ','Cr','Mn','Fe','Co','Ni','Cu','Zn',
     &'Fc','Ts','C2','Mc','S1','S2','As','Se','Rb','Sr',
     &'Y ','Zr','Nb','Mo','Pd','Ag','Cd','Sn','Sb','Te',
     &'Cs','Ba','Ce','Nd','Sm','Eu','Hf','Ta','W ','Pt',
     &'Au','Hg','Pb','Bi','Th','U ','La','Ga','$$','  '/
C ATWTOX CONTAINS OXIDE MOLE WEIGHTS NORMALIZED TO A SINGLE CATION
      DATA ATWTOX/
     &  9.007,   4.003,  14.938,  25.011,  34.809,
     & 44.009,  14.007,  15.999,  18.998,  20.183,
     & 30.990,  40.311,  50.980,  60.084,  70.971,
     & 80.061,  35.453,  39.948,  47.102,  56.079,
     & 68.954,  79.898,  90.939,  75.994,  70.937,
     & 71.846,  74.932,  74.709,  71.546,  81.369,
     & 79.845,  71.898,  67.995,  78.936,  32.064,
     & 32.064,  74.922,  78.960,  93.470, 103.619,
     &112.904, 123.218, 132.904, 143.937, 122.399,
     &115.870, 128.399, 150.688, 161.748, 127.600,
     &140.904, 153.339, 164.118, 168.238, 174.348,
     &175.958, 210.488, 220.945, 231.847, 211.089,
     &204.966, 216.589, 239.188, 248.978, 264.036,
     &270.028, 162.910,  93.720, 2*000.000/     !EXPANDED TO 68 ELEMENTS, 8
C NUMAT ARRAY CONTAINS ATOMIC NUMBERS OF ELEMENTS IN THE SAME SEQUENCE
C THAT THEY APPEAR IN ELNAM
      DATA NUMAT/
     &  1,  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,
     & 26, 22, 24, 25, 16, 16, 33, 34, 37, 38,
     & 39, 40, 41, 42, 46, 47, 48, 50, 51, 52,
     & 55, 56, 58, 60, 62, 63, 72, 73, 74, 78,
     & 79, 80, 82, 83, 90, 92, 57, 31, 2*0/
C ISITE ARRAYS CONTAIN ELEMENT CODES FOR EACH OF 4 PYROXENE SITES,
C THEREBY DEFINING THE PYROXENE COMPONENTS
      data isite1/
     &4*19,4*3,4*11,2*20,2*25,2*26,2*12,2*20,2*25,2*26,12,4*19,4*3,
     &4*11,7*20,7*25,7*26,7*12,7*20,4*25,4*30,4*26,3*12,25,30,8*40/
      data isite2/
     &12,28,26,33,12,28,26,33,12,28,26,33,8*22,12,26,12,26,12,26,12,
     &32,24,31,13,32,24,31,13,32,24,31,13,32,24,31,13,32,24,31,
     &32,24,31,13,32,24,31,   32,24,31,13,32,24,31,   32,24,31,13,
     &32,24,31,28,12,26,33,25,
     &30,20,28,12,26,33,28,12,26,33,28,12,33,26,28,33,12,25,30,8*40/
      data isite3/
     &12*22,13,31,13,31,13,31,13,31,
     &7*14,12*14,16*14,12*14,7*14,8*14,4*14,3*14,2*14,8*40/
      data isite4/
     &12*14,13,31,13,31,13,31,13,31,7*22,12*14,4*13,3*31,4*13,3*31,
     &4*13,3*31,4*13,3*31,7*14,4*14,4*14,4*14,3*14,2*14,8*40/
C NORDER ARRAY SPECIFIES THE ORDER IN WHICH PYROXENE NORMATIVE COMPONENTS
C ARE TO BE CALCULATED; THE CONTENTS ARE POSITIONS IN THE ISITE ARRAYS
      data norder/
```

```
     & 1, 3, 5, 7, 9,11,13,17,19,
     &14,18,20,21,22,27,26,28,29,30,31,32,33,34,35,36,37,38,39,40,41,
     &42,43,54,55,56,57,61,62,63,64,44,45,46,58,59,60,65,66,67,
     &71,85,88,68,83,87,80,81,73,76,77,72,74,86,89,2,4,6,8,10,12,15,
     &16,23,24,25,47,48,49,50,51,52,53,69,70,75,78,79,
     &82,84,90,91,8*88/
c IDCODE(X) IS THE POSITION OF EL X IN THE INPUT LIST
      data idcode/70*30/
C ITYPE ARRAY IS USED IN CONJUNCTION WITH THE ISITE ARRAYS
      data itype/
     &12*4, 8*2,5*3,2*7,
     &12*2,3*3,6,2*3,6,3*3,6,2*3,6,3*3,6,2*3,6,3*3,6,2*3,
     &6,6*2,1,11*2,1,2*2,1,2*1,8*8/
      end
```

Appendix III. Pyroxene norm components in the default order of calculation

	site 1	site 2	site 3	site 4	types
1	K	Mg	Ti	Si	4
2	K	Fe	Ti	Si	4
3	Li	Mg	Ti	Si	4
4	Li	Fe	Ti	Si	4
5	Na	Mg	Ti	Si	4
6	Na	Fe	Ti	Si	4
7	Ca	Ti	Al	Al	2
8	Fe	Ti	Al	Al	2
9	Mg	Ti	Al	Al	2
10	Ca	Ti	Fc	Fc	2
11	Fe	Ti	Fc	Fc	2
12	Mg	Ti	Fc	Fc	2
13	Ca	Mg	Si	Ti	3
14	Ca	Fe	Si	Ti	3
15	Mg	Mg	Si	Ti	7
16	Fe	Fe	Si	Ti	7
17	K	Ts	Si	Si	2
18	K	Cr	Si	Si	2
19	K	Fc	Si	Si	2
20	K	Al	Si	Si	2
21	Li	Ts	Si	Si	2
22	Li	Cr	Si	Si	2
23	Li	Fc	Si	Si	2
24	Li	Al	Si	Si	2
25	Na	Ts	Si	Si	2
26	Na	Cr	Si	Si	2
27	Na	Fc	Si	Si	2
28	Na	Al	Si	Si	2
29	Ca	Ts	Si	Al	3
30	Ca	Cr	Si	Al	3
31	Ca	Fc	Si	Al	3
32	Ca	Al	Si	Al	6
33	Fe	Ts	Si	Al	3
34	Fe	Cr	Si	Al	3
35	Fe	Fc	Si	Al	3
36	Fe	Al	Si	Al	6
37	Mg	Ts	Si	Al	3
38	Mg	Cr	Si	Al	3
39	Mg	Fc	Si	Al	3
40	Mg	Al	Si	Al	6
41	Ca	Ts	Si	Fc	3
42	Ca	Cr	Si	Fc	3
43	Ca	Fc	Si	Fc	6
44	Fe	Ts	Si	Fc	3
45	Fe	Cr	Si	Fc	3
46	Fe	Fc	Si	Fc	6

Appendix III--Con't.

	site 1	site 2	site 3	site 4	types
47	Mg	Ts	Si	Fc	3
48	Mg	Cr	Si	Fc	3
49	Mg	Fc	Si	Fc	6
50	Ca	C2	Si	Si	2
51	Fe	C2	Si	Si	2
52	Mg	C2	Si	Si	2
53	Ca	Ni	Si	Si	2
54	Fe	Ni	Si	Si	2
55	Mg	Ni	Si	Si	2
56	Zn	Mg	Si	Si	2
57	Zn	Fe	Si	Si	2
58	Ca	Zn	Si	Si	2
59	Mn	Mg	Si	Si	2
60	Mn	Fe	Si	Si	2
61	Ca	Mn	Si	Si	2
62	Ca	Ca	Si	Si	1
63	Fe	Fe	Si	Si	1
* 64	Mg	Mg	Si	Si	1
65	K	Ni	Ti	Si	4
66	K	C2	Ti	Si	4
67	Li	Ni	Ti	Si	4
68	Li	C2	Ti	Si	4
69	Na	Ni	Ti	Si	4
70	Na	C2	Ti	Si	4
71	Mn	Ti	Al	Al	2
72	Mn	Ti	Fc	Fc	2
73	Mn	Mg	Si	Ti	3
74	Mn	Fe	Si	Ti	3
75	Fe	Mg	Si	Ti	3
76	Mn	Ts	Si	Al	3
77	Mn	Cr	Si	Al	3
78	Mn	Fc	Si	Al	3
79	Mn	Al	Si	Al	6
80	Mn	Ts	Si	Fc	3
81	Mn	Cr	Si	Fc	3
82	Mn	Fc	Si	Fc	6
83	Ca	Mg	Si	Si	2
84	Ca	Fe	Si	Si	2
85	Mn	Ni	Si	Si	2
86	Mn	C2	Si	Si	2
87	Zn	Ni	Si	Si	2
88	Zn	C2	Si	Si	2
89	Fe	Mg	Si	Si	2
90	Mn	Mn	Si	Si	1
91	Zn	Zn	Si	Si	1

* Note: The default number of components to calculate is 64, any components below this point are not calculated unless they are chosen when ORDR is specified on the ****line.

Appendix IV. Arrays needed to change the order of the pyroxene component calculation

Array Position	isite 1	isite 2	isite 3	isite 4	itype
1	19 K	12 Mg	22 Ti	14 Si	4
2	19 K	28 Ni	22 Ti	14 Si	4
3	19 K	26 Fe	22 Ti	14 Si	4
4	19 K	33 C2	22 Ti	14 Si	4
5	3 Li	12 Mg	22 Ti	14 Si	4
6	3 Li	28 Ni	22 Ti	14 Si	4
7	3 Li	26 Fe	22 Ti	14 Si	4
8	3 Li	33 C2	22 Ti	14 Si	4
9	11 Na	12 Mg	22 Ti	14 Si	4
10	11 Na	28 Ni	22 Ti	14 Si	4
11	11 Na	26 Fe	22 Ti	14 Si	4
12	11 Na	33 C2	22 Ti	14 Si	4
13	20 Ca	22 Ti	13 Al	13 Al	2
14	20 Ca	22 Ti	31 Fc	31 Fc	2
15	25 Mn	22 Ti	13 Al	13 Al	2
16	25 Mn	22 Ti	31 Fc	31 Fc	2
17	26 Fe	22 Ti	13 Al	13 Al	2
18	26 Fe	22 Ti	31 Fc	31 Fc	2
19	12 Mg	22 Ti	13 Al	13 Al	2
20	12 Mg	22 Ti	31 Fc	31 Fc	2
21	20 Ca	12 Mg	14 Si	22 Ti	3
22	20 Ca	26 Fe	14 Si	22 Ti	3
23	25 Mn	12 Mn	14 Si	22 Ti	3
24	25 Mn	26 Fe	14 Si	22 Ti	3
25	26 Fe	12 Mg	14 Si	22 Ti	3
26	26 Fe	26 Fe	14 Si	22 Ti	7
27	12 Mg	12 Mg	14 Si	22 Ti	7
28	19 K	32 Ts	14 Si	14 Si	2
29	19 K	24 Cr	14 Si	14 Si	2
30	19 K	31 Fc	14 Si	14 Si	2
31	19 K	13 Al	14 Si	14 Si	2
32	3 Li	32 Ts	14 Si	14 Si	2
33	3 Li	24 Cr	14 Si	14 Si	2
34	3 Li	31 Fc	14 Si	14 Si	2
35	3 Li	13 Al	14 Si	14 Si	2
36	11 Na	32 Ts	14 Si	14 Si	2
37	11 Na	24 Cr	14 Si	14 Si	2
38	11 Na	31 Fc	14 Si	14 Si	2
39	11 Na	13 Al	14 Si	14 Si	2
40	20 Ca	32 Ts	14 Si	13 Al	3
41	20 Ca	24 Cr	14 Si	13 Al	3
42	20 Ca	31 Fc	14 Si	13 Al	3
43	20 Ca	13 Al	14 Si	13 Al	6
44	20 Ca	32 Ts	14 Si	31 Fc	3

Appendix IV--Con't.

Array Position	isite 1	isite 2	isite 3	isite 4	itype
45	20 Ca	24 Cr	14 Si	31 Fc	3
46	20 Ca	31 Fc	14 Si	31 Fc	6
47	25 Mn	32 Ts	14 Si	13 Al	3
48	25 Mn	24 Cr	14 Si	13 Al	3
49	25 Mn	31 Fc	14 Si	13 Al	3
50	25 Mn	13 Al	14 Si	13 Al	6
51	25 Mn	32 Ts	14 Si	31 Fc	3
52	25 Mn	24 Cr	14 Si	31 Fc	3
53	25 Mn	31 Fc	14 Si	31 Fc	6
54	26 Fe	32 Ts	14 Si	13 Al	3
55	26 Fe	24 Cr	14 Si	13 Al	3
56	26 Fe	31 Fc	14 Si	13 Al	3
57	26 Fe	13 Al	14 Si	13 Al	6
58	26 Fe	32 Ts	14 Si	31 Fc	3
59	26 Fe	24 Cr	14 Si	31 Fc	3
60	26 Fe	31 Fc	14 Si	31 Fc	6
61	12 Mg	32 Ts	14 Si	13 Al	3
62	12 Mg	24 Cr	14 Si	13 Al	3
63	12 Mg	31 Fc	14 Si	13 Al	3
64	12 Mg	13 Al	14 Si	13 Al	6
65	12 Mg	32 Ts	14 Si	31 Fc	3
66	12 Mg	24 Cr	14 Si	31 Fc	3
67	12 Mg	31 Fc	14 Si	31 Fc	6
68	20 Ca	28 Ni	14 Si	14 Si	2
69	20 Ca	12 Mg	14 Si	14 Si	2
70	20 Ca	26 Fe	14 Si	14 Si	2
71	20 Ca	33 C2	14 Si	14 Si	2
72	20 Ca	25 Mn	14 Si	14 Si	2
73	20 Ca	30 Zn	14 Si	14 Si	2
74	20 Ca	20 Ca	14 Si	14 Si	1
75	25 Mn	28 Ni	14 Si	14 Si	2
76	25 Mn	12 Mg	14 Si	14 Si	2
77	25 Mn	26 Fe	14 Si	14 Si	2
78	25 Mn	33 C2	14 Si	14 Si	2
79	30 Zn	28 Ni	14 Si	14 Si	2
80	30 Zn	12 Mg	14 Si	14 Si	2
81	30 Zn	26 Fe	14 Si	14 Si	2
82	30 Zn	33 C2	14 Si	14 Si	2
83	26 Fe	28 Ni	14 Si	14 Si	2
84	26 Fe	12 Mg	14 Si	14 Si	2
85	26 Fe	33 C2	14 Si	14 Si	2
86	26 Fe	26 Fe	14 Si	14 Si	1
87	12 Mg	28 Ni	14 Si	14 Si	2
88	12 Mg	33 C2	14 Si	14 Si	2
89	12 Mg	12 Mg	14 Si	14 Si	1
90	25 Mn	25 Mn	14 Si	14 Si	1
91	30 Zn	30 Zn	14 Si	14 Si	1