J KAU: Earth Sci., vol. 6, pp 99-112 (1413 A.H. / 1993 A.D.)

FECALC: A Basic Program for Determining the Fe^{3+} Concentration in Some Ferromagnesian Silicates and Oxides

I.Y. AL-FILALI
Faculty of Earth Sciences, King Abdulaziz University
Jeddah, Kingdom of Saudi Arabia

ABSTRACT. This paper gives a detailed description of a basic program for the calculation of Fe^{3+} concentration in pyroxene, amphibole, garnet and spinel depending on the electron microprobe data analysis.

The method of calculation is based on the equation derived by Droop (1987) which uses stoichiometric criteria assuming that iron is the only element present in the above-mentioned minerals with variable valency and oxygen is the only anion.

Introduction

Naturally, iron may occur in both the divalent and the trivalent states. However, Fe in the structure is strongly dependent on its valance state, and as electron microprobe analyses express iron as Fe^{2+} only, it is important to know the amount of Fe^{3+} in the cell as accurately as possible (Hawthorn 1982). Therefore, the problem of estimating Fe^{2+}/Fe^{3+} ratio in minerals from microprobe analyses has received much attention, particularly with respect to pyroxene, (Cawthorn and Collerson 1974, Brown and Bradshaw 1979 and Carpenter 1979).

Droop (1987) states that most of the published work on Fe^{3+} recalculation schemes are mineral-specific and usually applicable only to certain ranges of composition such as metamorphic sodic pyroxenes (Carpenter 1979). A general equation for estimating the Fe^{3+} content of oxides and silicates from microprobe analysis has been derived by Droop (1987). A hypercard computer program is presented by Mogessie *et al.* (1990) for amphibole formula calculation and nomenclature written on Apple Macintosh, based on the program of Mogessie and Tessadri (1982).

This paper describes a basic computer program for calculating the Fe^{3+} concentration in pyroxene, amphibole, garnet and spinel using the equation presented by Droop (1987) in the form:

$$F = 2\,x\,(1\text{-}T/S) \tag{1}$$

where F is the number of Fe^{3+} ions per x oxygen in the mineral formula, T is the ideal number of cations per formula unit, S is the observed cation total per x oxygen calculated assuming that all Fe to be Fe^{2+}.

Therefore, for the purpose of calculating Fe^{3+} in such minerals, equation (1) can be rewritten for pyroxene garnet and spinel as:

$$F = 12\,(1\text{-}4/s), \quad 0 = 6 \tag{2}$$

$$F = 24\,(1\text{-}8/s), \quad 0 = 12 \tag{3}$$

and

$$F = 64\,(1\text{-}24/s), \quad 0 = 32 \tag{4}$$

respectively. Calculation of Fe^{3+} in amphiboles is more complicated because of the possibility of vacant A sites. Depending on what assumptions are made about site occupancies, there are six different Fe^{3+} recalculation options available as illustrated by Robinson *et al.* (1982):

Option 1 : Total cations = 16 (all sites filled). This may be suitable for some alkali amphiboles.

Option 2 : Total cations = 15 exclusive of Na and K (Na and K are restricted to A site. Ca, Mg, Fe^{2+} and Mn zic permitted in M4 site). This option is suitable for Fe-Mg Mn amphiboles.

Option 3 : Total cations = 15 exclusive of K. (K is restricted to A site. Mg, Fe^{2+}, Mn, Ca and Na are permitted in M4 sites).

Option 4 : Total cations = 13 exclusive of K, Na and Ca. This option is suitable for calcic amphiboles.

Option 5 : Total Si to 8.

Option 6 : Total Si + Al to 8.

He suggested the assignment of cations into their structural positions in the unit cell as follows:

T sites : Add Si then Al to sum to 8.00.

M1, 2, 3 sites : Add left over Al, then Ti, Fe^{3+}, Cr^{3+}, Fe^{2+}, Zn, Mn, Ca, Li and Na in that order to sum to 5.00.

M4 sites : Add left over Mg, Fe^{2+}, Zn, Mn, Ca, Li and Na in that order to sum to 2.00.

A site : Add left over Ca, then Li, then K to sum not exceeding 1.00.

Hawthorne (1982) has divided the amphiboles into four principal groups on the basis of the cation occupancy as follows:

1 – (Ca + Na) M4 < 1.34 Fe-Mg-Mn group;

2 – (Ca + Na) M4 ≥ 1.34, (Na) < 0.67 } calcic amphiboles group;

3 – (Ca + Na) M4 ≥ 1.34, 0.67 < (Na) M4, ≤ 1.34 } sodic calcic amphiboles group;

4 – (Na) M4 ≥ 1.34 Alkali amphibole.

Program Description

The present program is written in Basic in an interactive style to provide wider distribution and easier utility employing most of the machines available in the laboratories. It is a menu driven program where a menu controls all the included functions through five different options. The functions are described in the flowchart (Fig. 1) while the program operations can be discussed in brief as follows:

A – Data Input

The microprobe analysis of any investigated mineral can be fed to the program using either the key board (option 1) or a disk file (option 2), by means of subroutines (KEYBRD) and (DSKFLE) respectively. The microprobe data are accepted in the element form where the analysed content of 10 major elements (Si, Ti, Cr, Al, Fe, Mn, Mg, Ca, Na, K) are provided. Besides, the values of oxygen (O) and iron oxides (FeO) are also requested by the program. Continuous printing of the input data is always monitored on the screen while a continuous print out is available if requested.

Fe_2 / Fe_3 Calculations

The calculation of the relative concentrations of the Fe^{2+} and Fe^{3+} is accomplished by the excution of Subroutine (FE2FE3) when option 3 is activated. The subroutine carries out this function, using the equation suggested by Droop (1987), in an automatic way without the interference of the user. However, when the investigated mineral belongs to the amphibole mineral group, the user should interfere to classify the mineral into one of the four amphibole subgroups (calcic, alkali, ...etc.) mentioned by Hawthorne (1982). The subroutine offers a suggested subgroup based on the relative occurrence of Ca and Na cations in the M4 site, however the final selection remains the choice of the user.

Cation Distribution of Amphiboles

The program pays some special attention to the amphibole minerals since they are considered to be of more complex composition which drew the interest of many investigators (e.g. Hawthorne 1982; Robinson *et al.* 1981; Droop 1987). In addition to the determination of the amphibole subgroup, as previously discussed, the program investigates the cation distribution of the analysed mineral in the different crystal sites. This operation is executed by Subroutine (AMPHCATION) which considers six crystal sites [A(0-1) M4(2) M1, 3(3) M2(2) T2(4) T1(4) O(22) OH, CI, F(2)] and can be activated through option 4.

Option 5 allows the user to terminate the program execution. The output of the

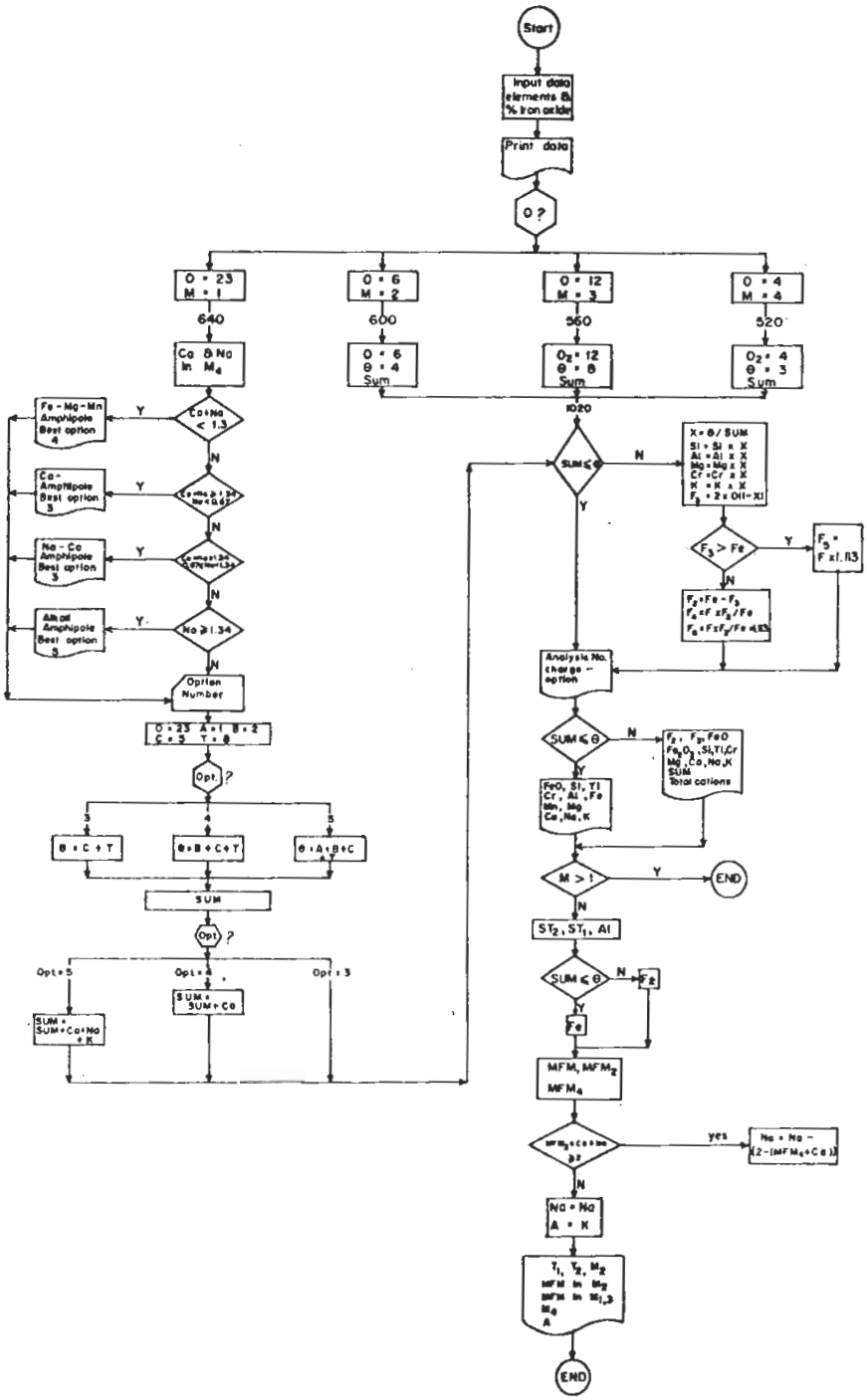

FIG. 1. A flowchart describing the function of the program.

different operations is available on both the screen and any line printer connected with the computer. The printed output sheets (Fig. 2) includes input data of microprobe mineral analysis, Fe^{2+}/Fe^{3+} recalculation, and amphibole cation distribution (for amphibole minerals). It is automatically processed during the execution of the different options allowed by the menu and do not require a separate option.

FIG. 2. Sodic-calcic amphibole.

```
  INPUT DATA :
  ============

 Analysis no. : DRP5.DAT

*=========================================================================*
*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !  K  *
* ------------------------------------------------------------------------ *
*7.1014 1.1391 0.1453 0.0000 0.0000 1.6111 0.0236 3.2267 0.8784 1.7058 0.4109 *
*=========================================================================*
      OXYGEN VAL.=  23           %FeO =  13.16
***************************************************************************

  OUTPUT DATA
  ===========

MINERAL GROUP IS : Amphibole
% FE-OXIDE =  13.16       FeO =  6.015121          Fe2O3= 7.940104
SUM =  13.2472      TOTAL CATIONS =  15.93921       OXYGEN NO. =  23.0002
*=========================================================================*
*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !  K  *
* ------------------------------------------------------------------------ *
*6.9689 1.1178 0.1426 0.0000 0.8584 0.7227 0.0232 3.1665 0.8620 1.6740 0.4032 *
*=========================================================================*

  MINERAL FORMULA
  ===============
  In Site T2:     TOTAL CATIONS=  4
  T2=4.0 Si
-------------------------------------------------------------------------

  In Site T1:     TOTAL CATIONS=  4
  T1=2.96888Si+1.03112Al
-------------------------------------------------------------------------

  In Site M2:     TOTAL CATIONS=  2
  M2=0.14259Ti+0.08673Al+0.85838Fe3+0.16851Fe2+0.00540Mn+0.73839Mg
-------------------------------------------------------------------------

  In Site M1,3:     TOTAL CATIONS=  3
  M1,3=0.55414Fe2+0.01776Mn+2.42810Mg
-------------------------------------------------------------------------

  In Site M4:     TOTAL CATIONS=  2
  M4=0.00000Fe2+0.00000Mn+0.00000Mg+0.86201Ca+1.13799Na
-------------------------------------------------------------------------

  In Site A:     TOTAL CATIONS=  .9392105
  A=0.53598Na+0.40323K
-------------------------------------------------------------------------

  TYPE OF AMPHIBOLE : SODIC-CALCIC Amphibole
=========================================
```

FIG. 2. Fe-Mn-Mg amphibole.

```
  INPUT DATA :
  ============

 Analysis no. : 0

*=============================================================================*
*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* -----------------------------------------------------------------------------*
*6.5206 2.3032 0.0535 0.0000 0.0000 1.2398 0.0280 4.5640 0.1298 0.2709 0.0000 *
*=============================================================================*
      OXYGEN VAL.=  23              %FeO =  10.673
*******************************************************************************


  OUTPUT DATA
  ============

MINERAL NAME IS : Amphibole
% FE-OXIDE =  10.673       FeO =  9.846031          Fe2O3= 1.141271
SUM =  15.0389      TOTAL CATIONS =  15.2702      OXYGEN NO. =  23.00005
*=============================================================================*
*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* -----------------------------------------------------------------------------*
*6.5037 2.4967 0.0534 0.0000 0.1190 1.1176 0.0279 4.5522 0.1295 0.2702 0.0000 *
*=============================================================================*
  MINERAL FORMULA
  ===============
  In Site T2:     TOTAL CATIONS=  4
  T2=4.0 Si
-------------------------------------------------------------------------------
  In Site T1:     TOTAL CATIONS=  4
  T1=2.50373Si+1.49627Al
-------------------------------------------------------------------------------
  In Site M2:     TOTAL CATIONS=  2
  M2=0.05336Ti+1.00046Al+0.11899Fe3+0.16225Fe2+0.00405Mn+0.66089Mg
-------------------------------------------------------------------------------
  In Site M1,3:     TOTAL CATIONS=  3
  M1,3=0.58845Fe2+0.01470Mn+2.39685Mg
-------------------------------------------------------------------------------
  In Site M4:     TOTAL CATIONS=  2
  M4=0.36690Fe2+0.00917Mn+1.49446Mg+0.12946Ca+0.00000Na
-------------------------------------------------------------------------------
  In Site A:     TOTAL CATIONS=  .2701984
  A=0.27020Na
-------------------------------------------------------------------------------

  TYPE OF AMPHIBOLE : FE-MN-MG Amphibole
=================================
```

FIG. 2. Garnet.

```
  INPUT DATA :
  ============

 Analysis no. : GT1.DAT

*=============================================================================*
*  Si   !  Al   !  Ti   !  Cr   ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* ------------------------------------------------------------------------- *
*2.9687 2.0043 0.0030 0.0000 0.0000 2.3090 0.0969 0.5598 0.0842 0.0000 0.0000 *
*=============================================================================*
      OXYGEN VAL.=  12            %FeO =  34.83
*****************************************************************************

  OUTPUT DATA
  ============

MINERAL GROUP IS : Garnet
% FE-OXIDE =  34.83        FeO =  33.65794          Fe2O3= 1.302514
SUM =  8.0259      TOTAL CATIONS =  8       OXYGEN NO. =  11.99975
*=============================================================================*
*  Si   !  Al   !  Ti   !  Cr   ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* ------------------------------------------------------------------------- *
*2.9591 1.9978 0.0030 0.0000 0.0774 2.2241 0.0966 0.5580 0.0839 0.0000 0.0000 *
*=============================================================================*
```

FIG. 2. Pyroxene.

```
  INPUT DATA :
  ============

 Analysis no. : PX1.DAT

*=============================================================================*
*  Si   !  Al   !  Ti   !  Cr   ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* ------------------------------------------------------------------------- *
*2.0126 0.4322 0.0019 0.0000 0.0000 0.2240 0.0009 0.3729 0.4726 0.5046 0.0000 *
*=============================================================================*
      OXYGEN VAL.=  6             %FeO =  7.45
*****************************************************************************

  OUTPUT DATA
  ============

MINERAL GROUP IS : Pyroxine
% FE-OXIDE =  7.45         FeO =  5.284851          Fe2O3= 2.40613
SUM =  4.0217      TOTAL CATIONS =  4       OXYGEN NO. =  5.999999
*=============================================================================*
*  Si   !  Al   !  Ti   !  Cr   ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* ------------------------------------------------------------------------- *
*2.0017 0.4299 0.0019 0.0000 0.0647 0.1580 0.0009 0.3709 0.4701 0.5019 0.0000 *
*=============================================================================*
```

FIG. 2. Spinel.

```
  INPUT DATA :
  ============

Analysis no. : SPI1.DAT

*=============================================================================*
*  Si   !  Al   !  Ti   !  Cr   ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* ------------------------------------------------------------------------- *
*0.0000 1.9870 0.0000 0.0000 0.0000 0.0980 0.0000 0.9160 0.0050 0.0000 0.0000 *
*=============================================================================*
      OXYGEN VAL.=  4            %FeO =  4.955
*****************************************************************************

  OUTPUT DATA
  ===========

MINERAL GROUP IS : Spinel
% FE-OXIDE =  4.955       FeO =  4.146007         Fe2O3= .8990336
SUM =  3.006      TOTAL CATIONS =  3       OXYGEN NO. =  3.999501
*=============================================================================*
*  Si   !  Al   !  Ti   !  Cr   ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
* ------------------------------------------------------------------------- *
*0.0000 1.9830 0.0000 0.0000 0.0160 0.0818 0.0000 0.9142 0.0050 0.0000 0.0000 *
*=============================================================================*
```

93/10/03
12:58:10

fecalc.bas

1

```
 10 REM PROGRAM FECALC
 20 DIM V1(8),V2(8),V3(8),V4(8),V5(8),U1$(8),U2$(8),U3$(8),U4$(8),U5$(8)
 30 DIM PNT(8),PT$(8),ST$(5),MN$(4),V(11)
 40 AM$(1)="FE-MN-MG" : AM$(2)="CALCIC" : AM$(3)="SODIC-CALCIC" : AM$(4)="ALKALI"
 50 ST$(1)="T1" : ST$(2)="M2" : ST$(3)="M1,3" : ST$(4)="M4" : ST$(5)="A"
 60 MN$(1)="Amphibole" : MN$(2)="Pyroxine" : MN$(3)="Garnet" : MN$(4)="Spinel"
 70 LN$="------------------------------------------------------------------------"
 80 SCREEN 0,1,0 : WIDTH 80 : COLOR 15,5,1 : CLS : KEY OFF : NS=5
 90 PRINT"          ************************************************"
100 PRINT"            P R O G R A M    F E - R E C A L C U L A T I O N"
110 PRINT"          ************************************************"
120 LOCATE 4,9 : PRINT"This program allows the user to do the following jobs:"
130 LOCATE 5,9 : PRINT"1- To recalculate the Fe2+/Fe3+ concentration in the
140 LOCATE 6,9 : PRINT"   the investigated mineral"
150 LOCATE 7,9 : PRINT"2- To determine the mineral group (pyroxene, amphibole,
160 LOCATE 8,9 : PRINT"   garnet or spinel) to which the mineral belongs.
170 LOCATE 9,9 : PRINT"3- In case of amphibole group, the program investigates"
180 LOCATE 10,9 : PRINT"   the amphibole subgroup and (e.g. calcic, alkali,..."
190 LOCATE 11,9 : PRINT"4- To perform the cation distribution for amphiboles"
200 LOCATE 12,9 : PRINT"A Basic program by Isam Y. Al Filali, FES, KAU, 1993"
210 LOCATE 13,9 :  PRINT"************************************************"
220 LOCATE 16,20 : PRINT"  ============================"
230 LOCATE 15,20 : PRINT"   O P E R A T I O N   M E N U"
240 LOCATE 16,20 : PRINT"  ============================"
250 LOCATE 17,20 : PRINT" 1- INPUT FROM KEYBOARD"
260 LOCATE 18,20 : PRINT" 2- INPUT OR STORE DATA FROM A DISKFILE"
270 LOCATE 19,20 : PRINT" 3- Fe2+/Fe3+ COMPUTATION"
280 LOCATE 20,20 : PRINT" 4- CATION DIST. IN AMPHIBOLE MINERALS"
290 LOCATE 21,20 : PRINT" 5- OUTPUT AND QUIT"
300 LOCATE 22,40 : INPUT"ENTER YOUR SELECTION:";OPT
310 ON OPT GOTO 510,330,830,1660
320 GOTO 2130
330 REM DSKFLE
340 CLS : PRINT" " : PRINT"  I/O USING A FILE" : PRINT"  ---------------"
350 INPUT "    INPUT FILE OR OUTPUT FILE ( I/O): ";Q$
360 IF Q$="O" THEN 440
370 INPUT "   ENTER INPUT FILENAME :",FL$
380 OPEN FL$ FOR INPUT AS #1
390 INPUT #1,AN$
400 INPUT#1,S1,TI,CR,AL,FE,MN,MG,CA,NA,K,O
410 INPUT#1,F
420 CLOSE#1 : INPUT"   PRINT INPUT DATA (Y/N) :"; Q0$
430 IF Q0$="Y" OR Q0$="y" THEN 630 ELSE GOTO 500
440 INPUT "  ENTER OUTPUT FILENAME :",FL$
450 OPEN FL$ FOR OUTPUT AS #2
460 PRINT #2,AN$
470 PRINT #2,SI,TI,CR,AL,FE,MN,MG,CA,NA,K,O
480 PRINT #2,F
490 CLOSE#2
500 INPUT"END OF DISKFILE OPERATION - PRESS ENTER TO CONTINUE ";O$ : GOTO 80
510 REM SUBPROGRAM KEYBRD
520 CLS : PRINT"  INPUT FROM KEYBOARD" : PRINT"   ---------------------"
530 PRINT" " : PRINT " " : INPUT "         ANALYSIS NUMBER ";AN$
540 INPUT "         DO YOU WANT RESULTS TO BE PRINTED ? Y/N  ",PT$ :PRINT
550 INPUT "  Si ";SI:INPUT "  Ti ";TI:INPUT "  Cr ";CR:INPUT "  Al ";AL:INPUT "  Fe ";FE
560 INPUT "  Mn ";MN:INPUT "  Mg ";MG:INPUT "  Ca ";CA:INPUT "  Na ";NA:INPUT "  K ";K
570 INPUT "  O ";O : INPUT "  % IRON OXIDE F";F
580 PRINT "   INPUT DATA :" : PRINT"   ----------"
590 PRINT "Si =";SI," Ti =";TI," Cr =";CR," Al =";AL," Fe =";FE
600 PRINT "Mn =";MN," Mg =";MG," Ca =";CA," Na =";NA,"  K =";K
610 IF(PT$="Y" OR PT$="y") THEN GOTO 630
620 GOTO 800
630 LPRINT"  INPUT DATA :" : LPRINT"  ==========="
640 PRINT"  INPUT DATA :" : PRINT"  ==========="
```

93/10/03 12:58:10 fecalc.bas 2

```
650 LPRINT" " : LPRINT" Analysis no. : ";AN$ : LPRINT" "
660 PRINT" " : PRINT" Analysis no. : ";AN$ : PRINT" "
670 LPRINT"*=============================================================================*"
680 PRINT"*-----------------------------------------------------------------------------*"
690 LPRINT"*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *"
700 PRINT"*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *"
710 LPRINT"* ------------------------------------------------------------------------- *"
720 PRINT"* ------------------------------------------------------------------------- *"
730 LPRINT"*"; : LPRINT USING"#.#### ";SI,AL,TI,CR,F3,FE,MN,MG,CA,NA,K;
740 PRINT"*"; : PRINT USING"#.#### ";SI,AL,TI,CR,F3,FE,MN,MG,CA,NA,K;
750 PRINT"*" : LPRINT"*"
760 LPRINT"*=============================================================================*"
770 PRINT"*-----------------------------------------------------------------------------*"
780 LPRINT"      OXYGEN VAL.= ";O; : LPRINT"          %FeO = ";F
790 PRINT"      OXYGEN VAL.= ";O; : PRINT"          %FeO = ";F
800 PRINT "*****************************************************************************"
810 LPRINT"*****************************************************************************"
: IF OPT=2 THEN 500
820 INPUT " END OF KEYBOARD INPUT-PRESS ENTER TO CONTINUE ";O$ : GOTO 80
830 REM SUBPROGRAM FE2FE3
840 CLS : PRINT"    Fe2+/Fe3+ RECALCULATION" : PRINT"   ----------------------"
850 PRINT"   CKECK THE LIST OF INVESTIGATED MINERAL GROUPS"
860 PRINT"   ------------------------------------------" : PRINT" "
870 PRINT "   1 - AMPHIPOLE  (O=23)" : PRINT "   2 - PYROXEN  (O=6)"
880 PRINT "   3 - GARNET  (O=12)" : PRINT "   4 - SPINEL  (O=4)"
890 IF(O=23) THEN 940
900 IF(O=6) THEN 960
910 IF(O=12) THEN 980
920 IF(O=4) THEN 1000
930 GOTO 1020
940 INPUT "IS IT AMPHIPOLE ?  YES/NO  ",AM$
950 IF(AM$="Y" OR AM$="y") THEN M=1 : GOSUB 1140
960 INPUT "IS IT PYROXEN ? YES/NO  ",PY$
970 IF(PY$="Y" OR PY$="y") THEN M=2 : GOSUB 1120
980 INPUT "IS IT GARNET ? YES/NO  ",G$
990 IF(G$="Y" OR G$="y") THEN M=3 : GOSUB 1100
1000 INPUT "IS IT SPINEL ? YES/NO  ",SP$
1010 IF(SP$="Y" OR SP$="y") THEN M=4 : GOSUB 1080
1020 INPUT "WHICH MINERAL GROUP ";M
1030 ON M GOSUB 1140,1120,1100,1080
1040 GOTO 1070
1050 PRINT "CODE OF DATA ENTRY IS WRRONG ?"
1060 PRINT "TRY AGAIN WITH F FROM FILE  OR K FROM KEYBOARD "
1070 END
1080 O=4 : THETA=3
1090 SUM=SI+NA+AL+MG+CA+K+FE+MN+TI+CR : GOSUB 1490 : RETURN : END
1100 O=12 : THETA=8
1110 SUM = SI+AL+MG+CA+FE+MN+TI+CR+K+NA : GOSUB 1490 : RETURN : END
1120 O=6 :THETA=4
1130 SUM=SI+NA+AL+MG+CA+FE+MN+TI : GOSUB 1490 : RETURN : END
1140 XX=SI+TI+CR+AL+FE+MN+MG
1150 IF(XX >= 13) THEN 1180
1160 CAA=13-XX
1170 CAB=CA-CAA : NAB=NA : GOTO 1230
1180 YY=XX-13
1190 ZZ=2-YY : CAB=CA
1200 IF(CAB >  ZZ) THEN NAB 0 : GOTO 1230
1210 NAB=ZZ-CAB
1220 IF(NAB > NA) THEN NAB=NA
1230 CNAM=CAB+NAB
1240 PRINT "IN M4 :  CA =";CAB;" ,  NA =";NAB;"   THUS   CA+NA  ";CNAM
1250 IF(CNAM < 1.34) THEN 1290
1260 IF((CNAM >= 1.34) AND (NAB < .67)) THEN 1300
1270 IF((CNAM >  1.34) AND (NAB >  .67 AND NAB < 1.34)) THEN 1320
```

93/10/03
12:58:10 **fecalc.bas** 3

```
1280 IF(NAB >= 1.34) THEN 1310
1290 LS=1 : PRINT"THIS IS FE-MG-MN AMPHIPOLE GROUP- BEST OPTION IS 4":GOTO 1330
1300 LS=2 : PRINT"THIS IS CALCIC-AMPHIPOLE GROUP- BEST OPTION IS 3" : GOTO 1330
1310 LS=4 : PRINT "THIS IS ALKALI AMPHIPOLE GROUP - BEST OPTION IS 5":GOTO 1330
1320 PRINT"THIS IS SODIC-CALCIC AMPHIPOLE GROUP-BEST OPTION IS 3": LS=3
1330 INPUT "OPTION NUMBER ";OP
1340 A=1 : B=2 : C=5 : T=8 : O=23
1350 IF (OP<3 OR OP>5) THEN PRINT "INVALID OPTION NO. TRY AGAIN":STOP
1360 IF OP=3 THEN 1390
1370 IF OP=4 THEN 1400
1380 IF OP=5 THEN 1410
1390 THETA=C+T : GOTO 1420
1400 THETA=B+C+T : GOTO 1420
1410 THETA=A+B+C+T
1420 SUM=SI+TI+AL+CR+FE+MN+MG
1430 IF OP=3 THEN GOSUB 1490 : RETURN
1440 IF OP=4 THEN 1460
1450 IF OP=5 THEN 1470
1460 SUM=SUM+CA : GOSUB 1490 : RETURN
1470 SUM=SUM+CA+NA+K
1480 GOSUB 1490 :RETURN
1490 IF SUM<=THETA THEN 1590
1500 X=THETA/SUM
1510 SI=SI*X : NA=NA*X : AL=AL*X : MG=MG*X : CA=CA*X : FE=FE*X
1520 MN=MN*X : TI=TI*X : CR=CR*X : K=K*X : F3=2*O*(1-X) : H=FE
1530 IF F3>FE THEN 1580
1540 F2=FE-F3 : H=F2
1550 F4=F*(F2/FE)
1560 F5=F*(F3/FE)*1.1113
1570 GOTO 1600
1580 F5=F*1.1113 : GOTO 1600
1590 F4=F : F5=0 : F2=FE : F3=0
1600 FE3=F3 : TNC = SI+NA+AL+MG+CA+K+F2+FE3+MN+TI+CR
1610 V(1)=SI : V(2)=AL : V(3)=TI : V(4)=CR : V(5)=FE3
1620 V(6)=F2 : V(7)=MN : V(8)=MG : V(9)=CA : V(10)=NA : V(11)=K
1630 OXN=2*SI+.5*NA+1.5*AL+MG+CA+.5*K+F2+1.5*FE3+MN+2*TI+1.5*CR
1640 INPUT"END OF Fe2-Fe3 CALCULATION, PRESS ENTER TO CONTINUE";O$
1650 GOTO 80
1660 REM SUBPROGRAM CATION DISTRIBUTION
1670 CLS : LOCATE 15,10
1680 IF M=1 THEN PRINT"CATION DISTRIBUTION FOR AMPHIBOLE " : GOTO 1700
1690 IF M>1 THEN PRINT"SORRY CATION DISTRIBUTION IS ONLY ALLOWED FOR AMPHIBOLE" : GOTO 212
0
1700 U1$(1) "Si" : U1$(2)="Al" : U5$(1)="Na" : U5$(2)="K"
1710 U2$(1)="Ti" : U2$(2)="Cr" : U2$(3)="Al" : U2$(4)="Fe3" : U2$(5)="Fe2"
1720 U2$(6)="Mn" : U2$(7)="Mg" : T2=4
1730 U3$(1)="Fe3" : U3$(2)="Fe2" : U3$(3)="Mn" : U3$(4) "Mg" : U3$(5)="Ca"
1740 U4$(1)="Fe2" : U4$(2)="Mn" : U4$(3)="Mg" : U4$(4)="Ca" : U4$(5)="Na"
1750 MFM=MG+H+MN : R1=MG/MFM : R2=H/MFM : R3=MN/MFM
1760 T1=SI-T2 : V1(1)= T1 : IF T1>=4 THEN 1800
1770 T1=T1+AL : IF T1<=4 THEN 1790
1780 DAL=T1-4 : V1(2)=AL-DAL : AL=DAL : GOTO 1800
1790 V1(2)=AL : AL=0
1800 M2=TI+CR+AL : V2(1)=TI : V2(2)=CR : V2(3)=AL : IF M2>=2 THEN 1890
1810 IF F3=0 THEN 1850
1820 M2=M2+F3 : IF M2<=2 THEN 1840
1830 DF3=M2-2 : V2(4)=F3-DF3 : F3=DF3 : GOTO 1890
1840 V2(4)=F3 : F3=0 : IF M2=2 THEN 1890
1850 M2=M2+MFM : IF M2<=2 THEN 1880
1860 DFM=M2-2 : FR=(MFM-DFM)/MFM : V2(5)=H*FR : V2(6)=MN*FR : V2(7)=MG
1870 H=H-V2(5) : MN=MN-V2(6) : MG=MG-V2(7) : MFM=DFM : GOTO 1890
1880 V2(5)=H : V2(6)=MN : V2(7)=MG : H=0 : MN=0 : MG=0 : MFM=0
1890 M13=0 : IF F3=0 AND MFM=0 THEN 1980
1900 IF F3=0 THEN 1920
```

93/10/03
12:58:10

fecalc.bas

4

```
1910 V3(1)=F3 : M13=F3 : F3=0 : IF M13>=3 THEN 2010
1920 M13=M13+MFM : IF M13<=3 THEN 1950
1930 DFM=M13-3 : FR=(MFM-DFM)/MFM : V3(2)=H*FR : V3(3)=MN*FR : V3(4)=MG*FR
1940 H=H-V3(2) : MN=MN-V3(3) : MG=MG-V3(4) : MFM=DFM : GOTO 2010
1950 V3(2)=H : V3(3)=MN : V3(4)=MG : H=0 : MN=0 : MG=0 : MFM=0
1960 IF M13=3 THEN 2010
1970 IF CA=0 THEN 2010
1980 M13=M13+CA : IF M13<=3 THEN 2000
1990 DCA=M13-3 : V3(5)=CA-DCA : CA=DCA : GOTO 2010
2000 V3(5)=CA : CA=0 : IF M13=3 THEN 2010
2010 IF MFM=0 THEN 2030
2020 M4=MFM : V4(1)=H : V4(2)=MN : V4(3)=MG : IF M4>=2 THEN 2110
2030 IF CA=0 THEN 2070
2040 M4=M4+CA : IF M4<=2 THEN  2060
2050 DCA=M4-2 : V4(4)=CA-DCA : CA=DCA : GOTO 2110
2060 V4(4)=CA : CA=0 : IF M4=2 THEN 2110
2070 IF NA=0 THEN 2110
2080 M4=M4+NA : IF M4<=2 THEN 2100
2090 DNA=M4-2 : V4(5)=NA-DNA : NA=DNA : GOTO 2110
2100 V4(5)=NA : NA=0
2110 A1=NA+K : V5(1)=NA : V5(2)= K
2120 LOCATE 17,10 : INPUT"END OF DISTRIBUTION ROUTINE, PRESS ENTER TO CONTINUE";O$ : GOTO
80
2130 REM SUBPROGRAM OUTPUT
2140 LPRINT" " : LPRINT"  OUTPUT DATA" : LPRINT"  ==========" : LPRINT" "
2150 PRINT" " : PRINT"  OUTPUT DATA :" : PRINT"  ==========" : PRINT" "
2160 LPRINT"MINERAL GROUP IS : "; MN$(M)
2170 PRINT"MINERAL GROUP IS : "; MN$(M)
2180 PRINT "% FE-OXIDE = ";F;"       FeO = ";F4;"         Fe2O3=";F5
2190 LPRINT "% FE-OXIDE = ";F;"      FeO = ";F4;"         Fe2O3=";F5
2200 LPRINT "SUM = ";SUM;"    TOTAL CATIONS = ";TNC;"     OXYGEN NO. = ";OXN
2210 PRINT "SUM = ";SUM;"    TOTAL CATIONS = ";TNC;"     OXYGEN NO. = ";OXN
2220 LPRINT"*=================================================================================*
"
2230 PRINT"*=================================================================================*"
2240 LPRINT"*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *
"
2250 PRINT"*  Si  !  Al  !  Ti  !  Cr  ! Fe3  ! Fe2  !  Mn  !  Mg  !  Ca  !  Na  !   K  *"
2260 LPRINT"* --------------------------------------------------------------------------- *
"
2270 PRINT"* --------------------------------------------------------------------------- *"
2280 LPRINT"*"; : PRINT"*";
2290 FOR I=1 TO 11
2300 LPRINT USING"#.#### ";V(I);
2310 PRINT USING"#.#### ";V(I);
2320 NEXT I
2330 LPRINT"*" : PRINT"*"
2340 LPRINT"*=================================================================================*
"
2350 PRINT"*=================================================================================*"
2360 IF M>1 THEN 2660
2370 CLS : LOCATE 3,4 : PRINT" MINERAL FORMULA" : PRINT"  ================"
2380 LPRINT" " : LPRINT"  MINERAL FORMULA" : LPRINT"  ==============="
2390 PRINT"  In Site T2:    TOTAL CATIONS=  4" : PRINT"  T2=4.0 Si" : PRINT LN$
2400 LPRINT"  In Site T2:    TOTAL CATIONS=  4" : LPRINT"  T2=4.0 Si" : LPRINT LN$
2410 FOR K=1 TO NS
2420 L=0 : SUMC=0
2430 FOR J=1 TO 8
2440 ON K GOTO 2460,2470,2480,2490
2450 V=V5(J) : U$=U5$(J) : GOTO 2500
2460 V=V1(J) : U$=U1$(J) : GOTO 2500
2470 V=V2(J) : U$=U2$(J) : GOTO 2500
2480 V=V3(J) : U$=U3$(J) : GOTO 2500
2490 V=V4(J) : U$=U4$(J)
```

93/10/03
12:58:10

fecalc.bas

5

```
2500 IF V=0 THEN 2520
2510 L=L+1 : PNT(L)=V : PT$(L)=U$ : SUMC=SUMC+V
2520 NEXT J
2530 PRINT"  In Site ";ST$(K);":"; : PRINT"    TOTAL CATIONS= ";SUMC : PRINT "  ";ST$(K);"
=";
2540 LPRINT"  In Site ";ST$(K);":"; : LPRINT"    TOTAL CATIONS= ";SUMC : LPRINT "  ";ST$(K
);"=";
2550 FOR I=1 TO L
2560 LPRINT USING"#.#####";PNT(I); : LPRINT PT$(I); : IF I<L THEN LPRINT"+";
2570 PRINT USING"#.#####";PNT(I); : PRINT PT$(I); : IF I<L THEN PRINT"+";
2580 NEXT I
2590 PRINT LN$ : LPRINT LN$
2600 NEXT K
2610 PRINT" " : LPRINT" "
2620 PRINT"  TYPE OF AMPHIBOLE : ";AM$(LS);" Amphibole"
2630 LPRINT"  TYPE OF AMPHIBOLE : ";AM$(LS);" Amphibole"
2640 PRINT"========================================"
2650 LPRINT"========================================"
2660 PRINT "  END OF OUTPUT ROUTINE " : INPUT"  PRESS ENTER TO CONT.";O$
2670 CLS : LOCATE 15,20 : PRINT" END OF PROGRAM"
2680 END
\032INT "  END OF OUTPUT ROUTINE " : INPUT"  PRESS ENTER TO CONT.";O$
```


Acknowledgement

For helpful discussion I am very grateful to Prof. Hamdy S. Sadek, Head of Geophysics department at Faculty of Earth Science, King Abdulaziz University, Saudi Arabia.

References

Brown, E.H. and **Bradshaw, J.Y.** (1979) Phase relations of pyroxene and amphibole in greenstone, blueschist and eclogite of Franciscan comples, California, Contribion of Mineralogy, *Petrology* **71:** pp. 67-84.

Carpenter, M.A. (1979) Omphacites from Greece, Turkey and Gautemala: composition limits of cation ordering, *American Mineralogist.* **64:** pp. 102-108.

Cawthorn, R.G. and **Collerson, K.D.** (1974) The recalculation of pyroxene end-member parameters and the estimation of ferrous and ferric iron content from electron microprobe analysis, *Ibid,* **59:** pp. 1203-1208.

Droop, G.T.R. (1987) A general equation for estimating Fe^{3+} concentrations in ferromagnesian silicates and oxides from microprobe analysis, using stoichiometric criteria, *Mineralogical Magazine* **51:** pp. 431-435.

Hawthorn, F.F. (1982) Crystal chemistry of the amphiboles. Chapter 1, *Reviews in mineralogy* Vol. **9A**. Mineralogical Society of America, pp. 1-102.

Mogessie, A., Tessadri, R. and **Veltman** (1990) EMP-AMPH – A hyper card program to determine the name of an amphibole from electron microprobe analysis according tot he international mineralogical association scheme, *Computers and Geosciences* **16**(3): pp. 309-330.

Mogessie, A. and **Tessadri R.** (1982) A basic computer program to determine the name of an amphibole from an electron microprobe analysis, *Geol. Paleont. Mitt. Inn-Sbruck* **11**(7): pp. 259-289.

Robinson, P., Spear, F.S., Schumacher, J.C., Laird, J., Klein, C., Evans, B.W. and **Doolan, B.L.** (1982) Phase relations of metamorphic amphiboles: Natural occurrence and theory. Chapter 1, *Reviews in mineralogy* Vol. **9B**. Mineralogical Society of America, pp. 1-227.

FECALC : برنـامـج بلغـة البِيْسِـك لتحـديد تركيز الحـديد الثلاثي في بعض السيليكات الحديدومغنيسية والأكاسيد

عصام يحيى الفيلالي

كلية علوم الأرض ، جامعة الملك عبد العزيز ، جـــدة ، المملكة العربية السعودية

المستخلص . يعـطي هذا البحث شرحًـا تفصيليًا لبرنـامج بلغة البِيْسِـك لحساب تركيز الحديد ثلاثي التكافؤ في معادن البيروكسين ، الأمفيبول ، الجارنت والسبنل . معتمدًا على البيانات المستخرجة من تحليل تلك المعادن بوساطة جهاز الميكروبروب .

وقد اعتمدت هذه العمليات الحسابية على المعادلة التي ذكرها Droop (1987) والتي اعتـبر فيها أن الحديد هو العنصر الوحيد في المعادن سابقة الذكر ذو التكافؤ المتعدد وأن الأكسجين هو الأنيون الوحيد .