Am-80-143

American Mineralogist, Volume 65, pages 1185–1191, 1980

Cation vacancies and the crystal chemistry of breakdown reactions in kimberlitic omphacites

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Abstract

The degree of alteration in clinopyroxenes from eclogitic inclusions in South African kimberlites is directly related to the deviation from stoichiometry of remnant unaltered areas in individual grains. Deviations from stoichiometry are reconciled by allowing up to 9 percent vacancy in the M2 site. The breakdown reaction accounting for the apparent alteration is:

$$Ca\,\square\,Al_2Si_4O_{12} \rightarrow CaAl_2SiO_6 + 3SiO_2$$

The products of this reaction are observed in X-ray precession photographs as a second Ca-Tschermak's pyroxene intergrown with the host omphacite plus quartz powder rings. I infer that a vacancy-containing pyroxene is stabilized by pressure but is highly unstable at lower pressures. A general FORTRAN program which breaks pyroxene compositions into end-members has been written to include a vacancy-containing end-member.

Introduction

In the course of mineralogical investigations of inclusions in South African kimberlite pipes, I noted that in eclogitic clinopyroxenes the apparent degree of breakdown closely correlates with the mineralogy of the specimen. Of the specimens observed, the kyanite- and coesite-bearing eclogites and grospydites exhibit the greatest degree of alteration, which appears as a cloudiness or white opacity in the clinopyroxenes. It is inferred that the alteration of these clinopyroxenes must have been extremely rapid and essentially isochemical, because coesite is preserved in one specimen in which the omphacitic pyroxene is quite altered (Smyth and Hatton, 1977; Smyth, 1977a). This led to the suspicion that a component in these pyroxenes is highly unstable at lower pressures, indeed much less stable than either jadeite or coesite.

In thin section, the alteration of the pyroxene appears fairly evenly distributed along very fine fractures (Fig. 1); however, small unaltered areas up to 50 μm in diameter remain throughout most grains. Also, the pyroxene appears unaltered where it occurs as inclusions up to 200 μm in diameter within coesite and garnet grains. Preliminary microprobe analyses of the unaltered areas showed that the pyroxenes contained Al^{VI} significantly in excess of Al^{IV} + Na + K, and had consistently and significantly fewer than 8.0 cations per 12.0 oxygens. A similar deviation from stoichiometry was noticed by Sobolev *et al.* (1968) in omphacites in kyanite eclogites from Siberian kimberlites, although no explanation was offered as to how such deviations might be maintained. O'Hara and Yoder (1967) reported anomalously high alumina in pyroxenes synthesized at 1500°C and 3.0 GPa (30 kbar), and suggested that there may be a solid solution toward kyanite. Thus, previous studies and the preliminary chemical data suggest that the deviations from stoichiometry might be responsible for the rapid breakdown of some of the omphacites, especially those from kyanite- and silica-bearing eclogites.

Wood and Henderson (1978) presented experimental evidence for substantial amounts of M-site vacancies in aluminous clinopyroxenes in the systems $CaAl_2SiO_6$–SiO_2 and $CaAl_2SiO_6$–$CaMgSi_2O_6$ at pressures of 25–32 kbar and temperatures of 1400–1500°C. They concluded that the non-stoichiometric pyroxene is stabilized by increased pressure and should be a stable component of natural clinopyroxenes, especially in the presence of excess SiO_2. My investigation was undertaken to document the existence and extent of the occurrence of vacancies in some natural jadeite-rich clinopyroxenes and to characterize the crystal chemistry of the breakdown

0003–004X/80/1112–1185$02.00

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      PROGRAM PYROS
C     PROGRAM TO CALCULATE PYROXENE NORMS BY METHOD OF ROSS 1976
C     PROGRAM WILL ADJUST FE2+/FE3+ TO ACHIEVE STOICHIOMETRY
C     PROGRAM WILL ALLOW UP TO 15% VACANCY IN M2
      DIMENSION ENDM(36),ENDW(36),ATWEM(36),ELT(15),ELO(15),ATW(15),
     1WTF(15),TITLE(18), ATOM(15),ELC(15),EMEM(4,36)
      DATA ATOM/'SI  ','ALIV','ALVI','TI  ','CR  ','FE3+','FE2+',
     1'MG  ','MN  ','CA  ','LI  ','NA  ','K   ','VAC.','O   '/
      DATA ATW/60.0848,50.9806,50.9806,79.8988,75.9987,79.8461,
     171.8464,40.3011,70.8374,56.0794,14.9387,30.9895,47.1017
     2,0.0001,15.9998   /
      DATA ATWEM/211.097,214.948,186.082,195.215,210.983,
     A227.148,230.999,202.133,
     1243.260,247.111,218.245,211.266,227.034,227.378,243.146,237.941,
     2222.173,253.700,243.142,227.374,258.900,246.993,231.225,262.760,
     3218.127,202.359,233.894,199.192,191.308,207.075,247.188,231
     4,420,212.955,232.330,200,794,263.864  /
      DATA EMEM/'LI C','R SI','2 06','    ','LI F','E SI',
     1'2 06','    ','LI A','L SI','2 06','    ','LI M','G/TI',' SI2',
     2' 06 ','LI K','E/TI',' SI2',' 06 ','NA C','R SI','2 06',
     3','NA F','E SI','2 06','    ','NA A','L SI','2 06','    ','NA M',
     4'G/TI','SI2 ',' 06 ','NA F','E/TI',' SI2',' 06 ','K CR',' SI ',
     5' 06 ','    ','K FE',' SI2',' 06 ','    ','K AL',' SI2',' 06
     6','    ','K MG','/TI ','SI2 ','06  ','K FE','/TI ','SI2 ','06  ',
     7'CA T','I AL','2 06','    ','MG T','I AL','2 06','    ','FE T',
     8'I AL','2 06','    ','CA C','R AL',' SI ','06  ','MG C',
     H'R AL',' SI ',
     9' 06 ','FE C','R AL',' SI ','06  ','CA F','E AL',' SI ','06  ',
     A'MG F','E AL',' SI ','06  ','FE F','E AL',' SI ',' 06 ',
     B'CA A','L AL',' SI ','06  ','MG A','L AL',' SI ',' 06 ',
     C'FE A','L AL',' SI ','06  ','CA.5',' AL ','SI2 ','06  ',
     D'MG.5',' AL ','SI2 ','06  ','FE.5',' AL ','SI2 ','06  ',
     E'CA N','N SI','2 06','    ','MN M','G SI','2 06','    ',
     F'MN F','E SI','2 06','    ','CA2 ','SI2 ','06  ','    ',
     G'MG2 ','SI2 ','06  ','    ','FE2 ','SI2 ','06  ','    '/
C      INITIALIZE
    2 WRITE (7,4)
    4 FORMAT(' PROGRAM TO CALCULATE PYROXENE END MEMBERS',
     1/'  TYPE 0 FOR ATOM NUMBER, 1 FOR OXIDE WEIGHT PERCENTS:')
      READ (5,8) INP
    8 FORMAT (I1)
      WRITE (7,10)
   10 FORMAT(' SPECIFY OUTPUT: (0=NO, 1=YES) CATION NUMBERS,
     1WEIGHT','PERCENT OXIDES (2I1):')
      READ (5,12) IOUT1,IOUT2
   12 FORMAT(2I1)
C--------INITIALIZE RUN
   30 CONTINUE
      DO 32 N=1,37
      ENDM(N)=0.0
   32 ENDW(N)=0.0
      DO 34 N=1,15
      ELT(N)=0.0
      ELC(N)=0.0
      ELO(N)=0.0
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```
   34 WTP(N)=0.0
      WTOT=0.0
      CAT1=0.0
      CAT2=0.0
      WEIGHT=0.0
      CATION=0.0
      WRITE(7,36)
   36 FORMAT(' ENTER TITLE (18A4)')
      READ (5,38) TITLE
   38 FORMAT(18A4)
      IF (INP.GT.0)GO TO 100
C--------ATOM IMPUT
      WRITE (7,52)
   52 FORMAT (' ENTER NUMBERS OF ATOMS FOR OXYGEN, SI, AND AL(IV)
     1  (3F6.4)')
      READ (5,54) ELT(15),ELT(1),ELT(2)
   54 FORMAT (3F6.4)
      WRITE (7,56)
   56 FORMAT(' ENTER AL (VI), TI, CR (3F6.4)')
      READ (5,54) ELT(3),ELT(4),ELT(5)
      WRITE (7,58)
   58 FORMAT (' ENTER FE2+, FE3+ (2F6.4):')
      READ(5,60) ELT(7),ELT(6)
   60 FORMAT(2F6.4)
      WRITE(7,62)
   62 FORMAT(' ENTER MG, MN (2F6.4):')
      READ(5,60)ELT(8),ELT(9)
      WRITE (7,64)
   64 FORMAT(' ENTER CA, LI (2F6.4):')
      READ(5,60)ELT(10),ELT(11)
      WRITE(7,66)
   66 FORMAT(' ENTER NA, K (2F6.4):')
      READ(5,60)ELT(12),ELT(13)
      DO 70 N=1,13
   70 CATION=CATION+ELT(N)
      ELT(3)=ELT(3)+ELT(2)
      GO TO 170
C-------OXIDE INPUT
C
  100 CONTINUE
      WRITE(7,102)
  102 FORMAT (' ENTER WEIGHT PERCENT OXIDES:',
     1/'   SIO2,  AL203  (2F6.4):')
      READ(5,60)WTP(1),WTP(3)
      WRITE(7,104)
  104 FORMAT(' ENTER   TIO2,  CR203 (2F6.4):')
      READ (5,60) WTP(4),WTP(5)
      WRITE(7,106)
  106 FORMAT ( ' ENTER  FEO,  FE203  (2F6.4):')
      READ(5,60) WTP(7),WTP(6)
      WRITE (7,108)
  108 FORMAT(' ENTER MGO,  MNO  (2F6.4):')
      READ(5,60)WTP(8),WTP(9)
      WRITE(7,110)
  110 FORMAT(' ENTER  CAO,  LI2O  (2F6.4):')
      READ(5,60)WTP(10),WTP(11)
```

```
      WRITE (7,112)
  112 FORMAT(' ENTER  NA2O,  K2O  (2F6.4):')
      READ(5,60) WTP(12),WTP(13)
      DO 140 N=1,13
  140 WTOT=WTOT+WTP(N)
      IF(WTOT.GT.00.0.AND.WTOT.LT.110.0) GO TO 150
      WRITE(7,144)
  144 FORMAT(' OXIDE TOTAL TOO LOW OR TOO HIGH!')
      GO TO 30
C
C--------CALCULATE CATION NUMBERS
C
  150 DO 160 N=1,13
      ELT(N)=WTP(N)/ATW(N)
  160 CATION=CATION+ELT(N)
      ELT(15)=CATION+ELT(1)+ELT(3)/2+ELT(4)+ELT(5)/2+ELT(6)/2
     1-ELT(11)/2-ELT(12)/2-ELT(13)/2
  170 DV1=6.0/ELT(15)
      DV2=4.0/CATION
      DO 172 N=1,15
      ELO(N)=ELT(N)*DV1
      ELC(N)=ELT(N)*DV2
  172 ELT(N)=ELT(N)*DV1
      ELT(2)=2.0-ELT(1)
      ELO(2)=2.0-ELO(1)
      ELC(2)=2.0-ELC(1)
      ELT(3)=ELT(3)-ELT(2)
      ELO(3)=ELO(3)-ELO(2)
      ELC(3)=ELC(3)-ELC(2)
      DO 174 N=1,13
      CAT2=CAT2+ELC(N)
  174 CAT1=CAT1+ELO(N)
C
C-------ADJUST FE2+, FE3+ RATIO FOR STOICHIOMETRY
C
      FE3AD=2.0*(6.0-ELC(15))
      IF(FE3AD.GT.ELC(7)) GO TO 186
      IF((FE3AD+ELC(6)).LT.0.0) GO TO 194
      ELC(6)=ELC(6)+FE3AD
      ELC(7)=ELC(7)-FE3AD
      ELC(15)=ELC(15)+FE3AD/2.0
      DO 182 N=1,15
      ELT(N)=ELC(N)
  182 ELO(N)=ELC(N)
      WRITE(7,184)
  184 FORMAT(' FE2+/FE3+ ADJUSTED FOR STOICHIOMETRY')
      GOTO 200
C-------ALL FE AS FE 3+
  186 ELC(6)=ELC(7)
      ELC(7)=0.0
      ELC(15)=ELC(15)+ELC(6)/2.0
      DO 188 N=1,13
  188 ELT(N)=ELC(N)
      ELO(6)=ELO(7)
      ELO(7)=0.0
      ELO(15)=ELO(15)+ELO(6)/2.0
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```
      DV1 ELO(15)/6.0
      DO 190 N=1,15
  190 ELO(N)=ELO(N)/DV1
      WRITE (7,192)
  192 FORMAT(' CATION TOTAL HIGH;  ALL FE AS FE3+')
      GO TO 200
C------CATION TOTAL LOW;  ALL FE AS FE2+
  194 ELO(7)=ELO(7)+ELO(6)
      ELO(6)=0.0
      ELO(14)=4.0-CAT1
      CAT1=4.0
      DO 196 N=1,15
      ELC(N)=ELO(N)
  196 ELT(N)=ELO(N)
      WRITE (7,198)
  198 FORMAT(' CATION TOTAL LOW;  ALL FE AS FE2+')
C
C------OUTPUT CATION TOTALS
C
  200 IF(IOUT1.LT.1)GO TO 230
      WRITE (7,202)
  202 FORMAT(' CATIONS  PER 6 OXYGENS   PER 4 CATIONS')
      DO 210 N=1,15
      IF(ELT(N).LE.0.0) GO TO 210
      WRITE (7,206)  ATOM(N),ELO(N),ELC(N)
  206 FORMAT(4X,A4,2(10X,F8.4))
  210 CONTINUE
      WRITE(7,212) CAT1,CAT2,CATION
  212 FORMAT(' TOTAL  ',3(10X,F8.4))
C
C-------RECALCULATE OXIDES
C
  230 IF(IOUT2.LT.1) GO TO 290
      DO 240 N=1,13
      WTP(N)=ELT(N)*ATW(N)
  240 WEIGHT=WEIGHT+WTP(N)
      DV3=WEIGHT/100.0
      DO 250 N=1,15
  250 WTP(N)=WTP(N)/DV3
C
C------OUTPUT OXIDE WEIGHT PERCENTS
C
      WRITE(7,272)
  272 FORMAT ('  WEIGHT PERCENT OXIDES')
      DO 276 N=1,13
  276 WRITE(7,274) ATOM(N),WTP(N)
  274 FORMAT(4X,A4,10X,F8.4)
  290 IF (ELT(3).GT.-0.002) GO TO 300
      WRITE(7,292) ELT(3)
  292 FORMAT(/' ANALYSIS INDICATES AL(VI) = 'F6.4,
     1'!!!'//)
C
C
C------CALCULATE PYROXENE END MEMBERS-----------------------------------
C
C
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  300 CONTINUE
      TOTW=0.0
      TOTM=0.0
      DO 390 N=1,3
      NN=10+N
      NM1=5*(N-1)+1
      NM2=5*(N-1)+2
      NM3=5*(N-1)+3
      IF(ELT(NN).LE.0.0) GO TO 390
C-------CR LIMITED
      IF(ELT(NN).LE.ELT(5)) GO TO 306
      ENDM(NM1)=ELT(5)
      ELT(5)=0.0
      ELT(NN)=ELT(NN)-ENDM(NM1)
      GO TO 310
C-------NN LIMITED
  306 ENDM(NM1)=ELT(NN)
      ELT(NN)=0.0
      ELT(5)=ELT(5)-ENDM(NM1)
      GO TO 390
C-------NN - FE3+ PYROXENES
  310 IF(ELT(6).LE.0.0) GO TO 320
      IF(ELT(NN).LE.ELT(6)) GO TO 316
C------FE3+ LIMITED
      ENDM(NM2)=ELT(6)
      ELT(6)=0.0
      ELT(NN)=ELT(NN)-ENDM(NM2)
      GO TO 320
C-------NN LIMITED
  316 ENDM(NM2)=ELT(NN)
      ELT(NN)=0.0
      ELT(6)=ELT(6)-ENDM(NM2)
      GO TO 390
C
C-------NN - AL(VI) PYROXENES
  320 IF(ELT(NN).LE.ELT(3)) GO TO 326
      IF(ELT(3).LE.0.0) GO TO 330
C-------AL LIMITED
      ENDM(NM3)=ELT(3)
      ELT(3)=0.0
      ELT(NN)=ELT(NN)-ENDM(NM3)
      GO TO 330
C------NN LIMITED
  326 ENDM(NM3)=ELT(NN)
      ELT(NN)=0.0
      ELT(3)=ELT(3)-ENDM(NM3)
      GO TO 390
C
C-------NN - MG/FE/TI PYROXENES
C
  330 DO 340 M=1,2
      MM=10-2*M
      NMM=NM3+M
      IF(ELT(NN).LE.ELT(4)/2.0.OR.ELT(NN).LE.ELT(MM)/2.0) GO TO 336
C-------MG/FE/TI LIMITED
      IF(ELT(4).LT.ELT(MM)) GOTO 332
```

```
C-------MG/FE LIMITED
        ENDM(NMM)=ELT(MM)/2.0
        ELT(MM)=0.0
        ELT(4)=ELT(4)-ENDM(NMM)/2.0
        ELT(NN)=ELT(NN)-ENDM(NMM)
        GO TO 340
C-------TI LIMITED
  332   ENDM(NMM)=ELT(4)*2.0
        ELT(4)=0.0
        ELT(MM)=ELT(MM)-ENDM(NMM)/2.0
        ELT(NN)=ELT(NN)-ENDM(NMM)
        GO TO 340
C-------NN LIMITED
  336   ENDM(NMM)=ELT(NN)
        ELT(NN)=0.0
        ELT(4)=ELT(4)-ENDM(NMM)/2.0
        ELT(MM)=ELT(MM)-ENDM(NMM)/2.0
        GO TO 390
  340   CONTINUE
        WRITE(7,342)
  342   FORMAT(' THERE IS EXCESS MONOVALENT CATION IN THIS PYROXENE')
  390   CONTINUE
        DO 392 N=1,15
  392   ELT(1)=ELT(1)-ENDM(N)*2.0
        IF(ELT(1).GT.0.0)GO TO 400
        WRITE (7,394)
  394   FORMAT(' RAN OUT OF SI IN MONOVALENT CATION REMOVAL')
        GO TO 900
C
C-------TI PYROXENES  (PASSAITES)
C
  400   DO 450 N=1,3
        NM=N+15
        IF(N.EQ.1)NN=10
        IF(N.EQ.2)NN=8
        IF(N.EQ.3)NN=7
        IF(ELT(2).LE.0.0.OR.ELT(4).LE.0.0)GO TO 500
        IF(ELT(NN).LT.(2.0*ELT(2)).OR.ELT(4).LT.(2.0*ELT(2)))
       1GO TO 410
C-------AL LIMITED
        ENDM(NM)=ELT(2)/2.0
        ELT(2)=0.0
        ELT(4)=ELT(4)-ENDM(NM)
        ELT(NN)=ELT(NN)-ENDM(NM)
        GO TO 500
C-------TI/MN LIMITED
  410   IF(ELT(NN).LT.ELT(4)) GO TO 420
C-------TI LIMITED
        ENDM(NM)=ELT(4)
        ELT(4)=0.0
        ELT(2)=ELT(2)-2.0*ENDM(NM)
        ELT(NN)=ELT(NN)-ENDM(NM)
        GO TO 500
C-------NN LIMITED
  420   ENDM(NM)=ELT(NN)
        ELT(NN)=0.0
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```
      ELT(2)=ELT(2)-2.0*ENDM(NM)
      ELT(4)=ELT(4)-ENDM(NM)
  450 CONTINUE
C
C-------TSCHERMAKS PYROXENES
C
  500 IF(ELT(2).LE.0.0)GO TO 600
      NM=18
      DO 580 N=1,3
      DO 570 M=1,3
      NM=NM+1
      IF(M.EQ.1)M2=10
      IF(M.EQ.2)M2=8
      IF(M.EQ.3)M2=7
      IF(N.EQ.1)M1=5
      IF(N.EQ.2)M1=6
      IF(N.EQ.3)M1=3
      IF(ELT(M1).LE.0.0)GO TO 580
      IF(ELT(M1).LE.ELT(2).OR.ELT(M2).LE.ELT(2))
     1GO TO 510
C------AL LIMITED
      ENDM(NM)=ELT(2)
      ELT(2)=0.0
      ELT(1)=ELT(1)-ENDM(NM)
      ELT(M1)=ELT(M1)-ENDM(NM)
      ELT(M2)=ELT(M2)-ENDM(NM)
      GO TO 600
C------M1/M2 LIMITED
  510 IF(ELT(M2).LE.ELT(M1))GO TO 520
C------M1 LIMITED
      ENDM(NM)=ELT(M1)
      ELT(M1)=0.0
      ELT(M2)=ELT(M2)-ENDM(NM)
      ELT(2)=ELT(2)-ENDM(NM)
      ELT(1)=ELT(1)-ENDM(NM)
      GO TO 580
C-------M2 LIMITED
  520 ENDM(NM)=ELT(M2)
      ELT(M2)=0.0
      ELT(M1)=ELT(M1)-ENDM(NM)
      ELT(1)=ELT(1)-ENDM(NM)
      ELT(2)=ELT(2)-ENDM(NM)
  570 CONTINUE
  580 NM=18+N*3
C
C-------VACENCY PYROXENES
C
  600 IF(ELT(14).LE.0.0)GO TO 650
      IF(ELT(3).LE.0.0)GO TO 640
      DO 630 N=1,3
      IF(N.EQ.1)M2=10
      IF(N.EQ.2)M2=8
      IF(N.EQ.3)M2=7
      NM=N+27
      IF(ELT(M2).LE.2.0*ELT(3).OR.ELT(14).LE.2.0*ELT(3))GO TO 610
C------AL LIMITED
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      ENDM(NM)=ELT(3)
      ELT(3)=0.0
      ELT(1)=ELT(1)-2.0*ENDM(NM)
      ELT(M2)=ELT(M2)-ENDM(NM)/2.0
      ELT(14)=ELT(14)-ENDM(NM)/2.0
      GO TO 640
C-------VACENCY LIMITED
  610 IF(ELT(M2).LE.ELT(14))GO TO 620
      ENDM(NM)=ELT(14)*2.0
      ELT(14)=0.0
      ELT(M2)=ELT(M2)-ENDM(NM)/2.0
      ELT(3)=ELT(3)-ENDM(NM)
      ELT(1)=ELT(1)-ENDM(NM)*2.0
       GO TO 650
C--------M2 LIMITED
  620 ENDM(NM)=ELT(M2)*2.0
      ELT(M2)=0.0
      ELT(14)=ELT(14)-ENDM(NM)/2.0
      ELT(3)=ELT(3)-ENDM(NM)
      ELT(1)=ELT(1)-ENDM(NM)*2.0
  630 CONTINUE
      GO TO 650
  640 WRITE(7,642)
  642 FORMAT(' TOO LITTLE AL FOR VACANCY, IS THERE ANY CR LEFT?')
C
C--------MN PYROXENES
C
  650 IF(ELT(9).LE.0.0)GO TO 700
      DO 680 N=1,3
      NM=N+30
      IF(N.EQ.1)M1=10
      IF(N.EQ.2)M1=8
      IF(N.EQ.3)M1=7
      IF(ELT(M1).LE.ELT(9)) GO TO 660
C-------MN LIMITED
      ENDM(NM)=ELT(9)
      ELT(9)=0.0
      ELT(M1)=ELT(M1)-ENDM(NM)
      ELT(1)=ELT(1)-ENDM(NM)*2.0
      GO TO 700
C-------M1 LIMITED
  660 ENDM(NM)=ELT(M1)
      ELT(M1)=0.0
      ELT(9)=ELT(9)-ENDM(NM)
      ELT(1)=ELT(1)-ENDM(NM)*2.0
  680 CONTINUE
C
C-------QUADRILATERAL PYROXENES
C
C-------WOLLASTONITE
  700 ENDM(34)=ELT(10)/2.0
      ELT(10)=0.0
      ELT(1)=ELT(1)-ENDM(34)*2.0
      IF(ELT(1).LE.0.0)GO TO 730
C-------ENSATITE
      ENDM(35)=ELT(8)/2.0
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      ELT(1)=ELT(1)-ELT(8)
      ELT(8)=0.0
      IF(ELT(1).LE.0.0)GO TO 730
C-------FERROSILITE
      ENDM(36)=ELT(7)/2.0
      ELT(1)=ELT(1)-ELT(7)
      ELT(7)=0.0
      IF(ELT(1).GE.-0.002)GO TO 800
C------INSUFFICIENT SI
  730 WRITE(7,732)ELT(1)
  732 FORMAT(' RAN OUT OF SI IN QUAD PYROXENES;  SI = ',F6.4)
C
C-------COMPUTE RATIOS
  800 DO 810 N=1,36
      ENDM(N)=ENDM(N)*100.
      TOTM=TOTM+ENDM(N)
      ENDW(N)=ENDM(N)*ATWEM(N)
  810 TOTW=TOTW+ENDW(N)
      DV1=TOTW/100.
      DO 812 N=1,36
  812 ENDW(N)=ENDW(N)/DV1
      QD=ENDM(34)+ENDM(35)+ENDM(36)
      WO=100.*ENDM(34)/QD
      EN=100.*ENDM(35)/QD
      FS=100.*ENDM(36)/QD
C
C-------OUTPUT
C
  900 WRITE(7,902)TITLE
  902 FORMAT(//1X,18A4,//' PYROXENE END MEMBER CALCULATIONS',
     1//' END MEMBER',6X,'MOLE PERCENT    WEIGHT PERCENT')
      DO 904 N=1,36
      IF(ENDM(N).EQ.0.0)GO TO 904
      WRITE(7,906)EMEM(1,N),EMEM(2,N),EMEM(3,N),
     1EMEM(4,N),ENDM(N),ENDW(N)
  904 CONTINUE
  906 FORMAT(2X,4A4,2(4X,F8.3))
      WRITE(7,908) TOTM
  908 FORMAT(/' TOTAL',16X,F8.3,6X,'100.000')
C-------RESIDUALS
      DO 920 N=1,14
      IF(ELT(N).LT.0.001.AND.ELT(N).GT.-0.001) GO TO 920
      WRITE(7,918)ATOM(N),ELT(M)
  918 FORMAT(' RESIDUAL  ',A4,F8.3)
  920 CONTINUE
      WRITE(7,922) WO,EN,FS
  922 FORMAT(' QUADRILATERAL COORDINATES (MOLE PERCENTS):',
     1//' WO = ',F6.2,',   EN = ',F6.2,',   FS =  ',F6.2///)
      GO TO 30
      CALL EXIT
      END
```