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

JOSEPH R. SMYTH

Geosciences Division, Los Alamos Scientific Laboratory
Los Alamos, New Mexico 87545

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:

\[
\text{Ca}^{2+} \text{Al}_2\text{Si}_4\text{O}_{12} \rightarrow \text{CaAl}_2\text{Si}_6\text{O}_{18} + 3\text{SiO}_2
\]

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 gosspydites 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 isochronal, 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 \(\mu\)m in diameter remain throughout most grains. Also, the pyroxene appears unaltered where it occurs as inclusions up to 200 \(\mu\)m in diameter within coesite and garnet grains. Preliminary microprobe analyses of the unaltered areas showed that the pyroxenes contained \(\text{Al}^{IV}\) significantly in excess of \(\text{Al}^{IV} + \text{Na} + \text{K}\), 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$_2$Si$_2$O$_6$-SiO$_2$ and CaAl$_2$Si$_2$O$_6$-CaMgSi$_2$O$_6$ 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.
PROGRAM PYROS
PROGRAM TO CALCULATE PYROXENE NORMS BY METHOD OF ROSS 1976
PROGRAM WILL ADJUST FE2+/FE3+ TO ACHIEVE STOICHIOMETRY
PROGRAM WILL ALLOW UP TO 15% VACANCY IN M2
DIMENSION ENDM(36), ENDW(36), ATWEN(36), ELT(15), ELO(15), ATM(15),
1WTP(15), TITLE(18), ATOK(15), ELCK(15), EMEM(4,36)
DATA ATOK,'SI ','ALIV','ALVI','TI ','CR ','FE3+','FE2+
1'MG ',' Mn ','CA ','LI ','NA ','K ','VAC','0 '
DATA ATW/40. 0843,50.9306,50.9306,79.8983,75.9987,79.8461,
171.8464,40. 3011,70.8374,56.0794,14.9387,30.9895,47.1017
2.0. 0001,15.9998 /
DATA ATWEN/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,
2222.173,253.700,243.142,227.374,258.900,246.973,231.225,262.760,
3218.127,202.359,233.894,199.192,191.308,207.075,247.188,231
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 ','SI 2',
2.06,'LI M ','E/TI ','SI 2',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 ','SI 2',06,'NA F ','E/TI ','SI 2',06,'K CR ','SI ',
5.'K FE ','SI 2',06,'K AL ','SI 2',06,
6.'K MG ','/TI ','SI 2',06,'K FE ','/TI ','SI 2',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 ','A I ','06','MG C ',
9.'R AL ','SI ',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 .A ','L AL ','SI ',06
D.'MG.S ','AL ','SI 2',06,'FE S ','AL ','SI 2',06
E.'CA N ','N SI ','2.06','NN M ','G SI ','2.06
F.'MN F ','E SI ','2.06','CA2 ','SI 2',06
G.'MG2 ','SI 2',06,'FE 2 ','SI 2',06

C INITIALIZE
2 WRITE (7,4)
4 FORMAT(' PROGRAM TO CALCULATE PYROXENE END MEMBERS',
1/' TYPE 0 FOR ATON NUMBER, 1 FOR OXIDE WEIGHT PERCENTS!')
READ (5,8) INF
8 FORMAT (11)
WRITE (7,10)
10 FORMAT(' SPECIFY OUTPUT: (0=NO, 1=YES) CATION NUMBERS,'
1 WEIGHT', 'PERCENT OXIDES (2TI)!'')
READ (5,12) IDOUT1,IDOUT2
12 FORMAT(211)
C-----INITIALIZE RUN
30 CONTINUE
32 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
34 CONTINUE
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 (INF,GT,0) GO TO 100

C-------ATOM INPUT

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, OR (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(9)
WRITE (7,64)
64 FORMAT(' ENTER CA, Li (2F6.4)'
READ (5,60) ELT(11)
WRITE (7,66)
66 FORMAT(' ENTER NA, K (2F6.4)'
READ (5,60) 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, AL2O3 (2F6.4)'
READ (5,60) WTP(1), WTP(3)
WRITE (7,104)
104 FORMAT(' ENTER TI02, CR2O3 (2F6.4)'
READ (5,60) WTP(4), WTP(5)
WRITE (7,106)
106 FORMAT(' ENTER FEO, FE2O3 (2F6.4)'
READ (5,60) WTP(7), WTP(6)
WRITE (7,108)
108 FORMAT(' ENTER NGO, KNO (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 NA2Ov K2O (2F6.4):')
READ(5, 60) WTP(12), WTP(13)
DO 140 N=1, 13
140 WTP(N)=WTP(N)/WTP(N)
IF(WTP(GT.00.0, AND, WTP(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 196
IF(FE3AD+ELC(6), LT.0.0) GO TO 194
ELC(4)=ELC(4)+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')
GO TO 200
C
C--------ALL FE AS FE 3+
C
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
ELC(15)=ELC(15)+ELO(7)
DVI = ELO(15)/6.0
DO 190 N=1,15
190 ELO(N)=ELO(N)/DVI
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
.
200 IF(IOU1.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,F6.4))
210 CONTINUE
WRITE(7,212) CAT1,CAT2,CATION
212 FORMAT(’ TOTAL ’,3(10X,F8.4))
C
C-------RECALCULATE OXIDES
.
230 IF(IOU2.LT.1)GO TO 290
DO 240 N=1,13
WTP(N)=ELT(N)*ATM(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
.
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-------CALCULATE PYROXENE END MEMBERS-----------------------------------
C
C
C
CONTINUE
TOI=H=0.0
TOJ=T=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
315 ENDM(NM2)=ELT(NN)
ELT(NN)=0.0
ELT(6)=ELT(6)-ENDM(NM2)
GO TO 390
C
C---NN - AL(V1) 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 - KG/FE/TI PYROXENES
C
330 DD 340 M=1,2
MM=10-2*M
NMM=NM3+M
IF(ELT(NN),LE.,ELT(4)/2.0,OR.,ELT(NN),LE.,ELT(NM)/2.0) GO TO 336
C---MB/FE/TI LIMITED
IF(ELT(4),LT.,ELT(NN)) GOTO 332
C------MG/FE LIMITED
   ENDM(NMM) = ELT(NM)/2.0
   ELT(NM) = 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(NM) = ELT(NM) - 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(NM) = ELT(NM) - 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 (FASSAITES)
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)))
     GO 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
ELT(2) = ELT(2) - 2.0*ENDM(NM)
ELT(4) = ELT(4) - ENDM(NM)

450 CONTINUE

C

C-------TSCHERMAK'S 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(K1) = 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(K1) = 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-------VACANCY 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
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------ VACANCY 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------ K2 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------ 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------ QUADRILATERAL PYROXENES

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
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 ------- 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)
   WD = 100.0 * ENDM(34) / QD
   EN = 100.0 * ENDM(35) / QD
   FS = 100.0 * ENDM(36) / QD

C ------- OUTPUT

C
900 WRITE(7, 902) TITLE
902 FORMAT( ' PYROXENE END MEMBER CALCULATIONS',
           ' END MEMBER', ' MOLE PERCENT', ' WEIGHT PERCENT')
   DO 904 N = 1, 36
      IF(ENDM(N) .EQ. 0.0) GO TO 904
      WRITE(7, 906) ENM(1, N), ENM(2, N), ENM(3, N),
                   EMEM(4, N), ENDM(N), ENDW(N)
904 CONTINUE
906 FORMAT( ' TOTAL', 16X, '100.000')
   WRITE(7, 908) TOTM
908 FORMAT( ' QUADRILATERAL COORDINATES (MOLE PERCENTS):',

920 CONTINUE
   WRITE(7, 922) WD, EN, FS
922 FORMAT( ' QUADRILATERAL COORDINATES (MOLE PERCENTS):',
GO TO 30
CALL EXIT
END