MANTLE: A PROGRAM TO CALCULATE A 30 kbar NORM ASSEMBLAGE

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Abstract—MANTLE is a FORTRAN IV code to calculate mineral assemblages which would be expected at a pressure of 30 kbars from a bulk composition given in nine oxide components. The program also calculates the theoretical STP bulk density of the assemblages, and has been used for modeling mantles of the terrestrial planets.

With some improvements it may prove useful in modeling the upper mantle of the earth.

Key Words: Geochemistry, Mantle, Mars, Mineralogy, Planetology.

INTRODUCTION

In order to model the interiors of terrestrial planets, a FORTRAN IV program MANTLE was written to calculate a mineral assemblage and theoretical STP bulk density to be expected at 30 kbars (3.0 GPa) for a given rock composition. It is written for interactive calculations on DEC PDP-11 series computers using the RT-11 operating system. The nine oxide components required for input are SiO₂, Al₂O₃, TiO₂, MgO, FeO, Fe₂O₃, CaO, Na₂O, and K₂O. The program casts the analyses into anhydrous phases which are known to be stable at 25–35 kbar and 900–1300°C. The calculated phases correspond roughly to those observed in mantle-derived inclusions in kimberlites and basalts. The range of compositions accepted by the program exceeds that observed in terrestrial samples from high pressure origins. In situations where observational and thermodynamic data that would define stable phase assemblages are lacking, a few assumptions are made concerning such a phase assemblage.

The program was written to predict physical properties (especially densities) and mineral assemblages for various bulk compositions. It has proved useful in the modeling of terrestrial planets. It was used extensively to derive densities from trial compositions, and to predict partial melt compositions from calculated assemblages in modeling a hypothetical upper mantle for Mars (McGetchin and Smyth, 1978). The 30 kbar pressure corresponds to a depth of 250 km in Mars, 90 km in Earth and Venus, 350 km in Mercury, and 500 km in the Moon, and so it is hoped that the program will be useful for modeling the upper mantle and all of the terrestrial planets. I have received several requests for copies of the program since the work of McGetchin and Smyth (1978), and feel publication of the program may lead to refinements of the algorithm and possibly to some needed investigations in experimental petrology.

ALGORITHM

Figure 1 is a flowchart of the algorithm. The oxide components are input as weight percents of SiO₂, TiO₂, Al₂O₃, MgO, FeO, Fe₂O₃, CaO, Na₂O, and K₂O, which are converted immediately to relative numbers of cations. The first step is to remove Ti because it is assumed not to enter the silicate phases. Ti is removed either as rutile (TiO₂) or if Ti exceeds Fe²⁺, or as ilmenite (FeTiO₃) if Fe²⁺ exceeds Ti, as is usual. The second step is to remove K as a hypothetical pyroxene KAl₂Si₂O₈. This is a bit arbitrary and is based on occurrence of pyroxenes containing up to 1.2 weight percent K₂O as inclusions in diamonds (Rickard and Smyth, 1979, unpubl.). Compositions with K in excess of either Al or 2 x Si are rejected as implausible.

The next step is to calculate ratios of Mg to Fe²⁺ and Al to Fe²⁺ for partitioning between various phases. All phases are assumed to have equal ratios of Mg to Fe²⁺ and Al to Fe²⁺. Na is the next cation to be removed; as the pyroxenes, jadeite and acmite, in the ratio Al to Fe²⁺, respectively. Compositions with Na in excess of Al + Fe²⁺ are rejected as being too alcalic. The remaining Fe²⁺ then is removed as andradite garnet (Ca₃Fe²⁺₂Si₃O₁₂), with rejection if Fe²⁺ exceeds 1.5 times Ca or 1.5 times Si.

After removal of andradite, all remaining compositions are accepted and a major branch occurs based on the ratio of Ca to Fe²⁺ + Mg. If Ca exceeds Mg + Fe²⁺, the program branches to Ca-rich assemblages. Few, if any, of these assemblages have been recognized in terrestrial samples, or hypothesized for extraterrestrial occurrences, and will not be dealt with further here, but are included in the program for completeness. The Ca-poor branch leads to the more common eclogite and peridotite assemblages.

The next step in this branch is to remove the Ca as the clinopyroxenes, diopside, and hedenbergite, in the ratio of Mg to Fe²⁺. Then the path branches on the ratio of Al to Mg + Fe²⁺. On the Al-rich branch, there is a second branch to Si-rich and Si-poor compositions. In the Si-poor branch, pyrope (Mg₃Al₂Si₃O₁₂) and almandine (Fe₃Al₂Si₃O₁₂) garnets are removed, and the remainder then is Si-free with aluminum greater than twice the Mg + Fe. Spinel (MgAl₂O₄) and hercynite (FeAl₂O₄) then are removed according to the Mg to Fe²⁺ ratio, and the remaining excess alumina is assigned to corundum (path...
Figure 1. Flowchart of algorithm to compute a 30 kbar normative mineral assemblage. Path members (1-7) are discussed in text.
1. In the Si-rich branch, pyrope and almandine also are removed, but here the residuum is depleted in Mg and Fe, containing only silica and alumina. Kyanite then is removed until the residuum is depleted in either silica or alumina, and the residual silica or alumina are assigned to coesite (path 2) or coronand (path 3). Eclogite inclusions in kimberlites typically follow paths 1, 2, or 3.

After removal of diopsode–hedenbergite, the Al-poor, Mg-Fe-rich branch to paths 4–7 includes the mineralogies of the usual peridotites. Path 4 is followed by compositions in which $3 \times Al$ exceeds $2 \times Si$, and removal of garnet is limited by silica. The residuum here contains $Mg + Fe$ in excess of $1/2 \times Al$, so that spinel–hercynite is removed, leaving residual MgO + FeO which are assigned to periclase–wustite. Paths 5, 6, and 7 are perhaps more typical of terrestrial compositions, with the vast majority of peridotites following path 6. Path 5 is followed by low-silica compositions leaving periclase–wustite as a residual phase, and is discussed in a later section. Path 6 is followed by intermediate silica compositions, resulting in an orthopyroxene-olivine assemblage. Silica-rich compositions would follow path 7, resulting in all Mg + Fe forming orthopyroxenes and residual silica forming coesite. Such assemblages are unknown terrestrially.

The program then computes the theoretical STP density of the assemblage based upon the partial molar volumes of each phase. The program thus assumes that each mineral component exists as a separate phase, or that mixing between end members is ideal. The densities at STP are given in Table 1. The output lists only the end-members present, and gives mole and weight percents for each.

### Table 1. Norm minerals and STP densities used in program MANTLE

<table>
<thead>
<tr>
<th>Mineral</th>
<th>STPDensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clinopyroxenes</td>
<td></td>
</tr>
<tr>
<td>K-Jadeite</td>
<td>NaAlSi$_2$O$_6$</td>
</tr>
<tr>
<td>Jadeite</td>
<td>NaAlSi$_2$O$_6$</td>
</tr>
<tr>
<td>Acmite</td>
<td>NaFeSi$_2$O$_6$</td>
</tr>
<tr>
<td>Diopsode</td>
<td>CaMgSi$_2$O$_6$</td>
</tr>
<tr>
<td>Hedenbergite</td>
<td>CaFeSi$_2$O$_6$</td>
</tr>
<tr>
<td>Wallastonite</td>
<td>CaSi$_2$O$_6$</td>
</tr>
<tr>
<td>Orthopyroxenes</td>
<td></td>
</tr>
<tr>
<td>Enstatite</td>
<td>Mg$_2$Si$_2$O$_6$</td>
</tr>
<tr>
<td>Ferrosilite</td>
<td>Fe$_2$Si$_2$O$_6$</td>
</tr>
<tr>
<td>Ollivines</td>
<td></td>
</tr>
<tr>
<td>Forsterite</td>
<td>Mg$_2$SiO$_4$</td>
</tr>
<tr>
<td>Fayalite</td>
<td>Fe$_2$SiO$_4$</td>
</tr>
<tr>
<td>Monticellite</td>
<td>CaMgSiO$_4$</td>
</tr>
<tr>
<td>Kirschsteinite</td>
<td>CaFeSiO$_4$</td>
</tr>
<tr>
<td>Garnets</td>
<td></td>
</tr>
<tr>
<td>Andradite</td>
<td>Ca$_2$Fe$_2$Si$_2$O$_6$</td>
</tr>
<tr>
<td>Pyrope</td>
<td>Mg$_2$Al$_2$Si$_2$O$_6$</td>
</tr>
<tr>
<td>Almandine</td>
<td>Fe$_2$Al$_2$Si$_2$O$_6$</td>
</tr>
<tr>
<td>Grossular</td>
<td>Ca$_2$Al$_2$Si$_2$O$_6$</td>
</tr>
<tr>
<td>Oxides, Spinels, and Alumino-silicates</td>
<td></td>
</tr>
<tr>
<td>Periclase</td>
<td>MgO</td>
</tr>
<tr>
<td>Wustite</td>
<td>FeO</td>
</tr>
<tr>
<td>Rutile</td>
<td>TiO$_2$</td>
</tr>
<tr>
<td>Ilmenite</td>
<td>FeTiO$_3$</td>
</tr>
<tr>
<td>Coesite</td>
<td>SiO$_2$</td>
</tr>
<tr>
<td>Corundum</td>
<td>Al$_2$O$_3$</td>
</tr>
<tr>
<td>Calcite</td>
<td>CaO</td>
</tr>
<tr>
<td>Kyanite</td>
<td>Al$_2$SiO$_5$</td>
</tr>
<tr>
<td>Spinel</td>
<td>MgAl$_2$O$_4$</td>
</tr>
</tbody>
</table>

$^1$Estimated based on cell volume = 430 A$^3$
$^2$Clark et al., 1969
$^3$Robie et al., 1964
$^4$Sueno et al., 1973

### DISCUSSION

The algorithm described previously is the first step toward predicting mineralogies at 30 kbar, and there are many methods in which the program can be improved. However, the program works well for typical terrestrial compositions. The density calculations seem to be good enough for modeling purposes and are not likely to be greatly affected by minor changes in mineralogy.

The program has pointed up the need for some additional investigations in experimental petrology. In the low-silica compositions inferred for Mars by McGetchin and Smyth (1978), a significant uncertainty arises over the low-silica phase which would appear as orthopyroxene disappears on the addition of FeO to "pyrolite" composition of (Ringwood, 1964). Using a single observation of periclase–wustite (78% MgO) in an inclusion in a natural diamond (Rickard and Smyth, 1979, unpubl.). It has been assumed that periclase is the stable low-silica phase in the presence of olivine, clinopyroxene, and garnet. This assumption is rather arbitrary, and spinel or monticellite are equally likely as the fourth phase. These low-silica compositions have not been investigated adequately experimentally in this pressure range, and there are insufficient thermodynamic data to predict the stable assemblage, even for the iron-free system. In particular, the three reactions between the following three four-phase assemblages

\[
\begin{align*}
\text{Periclase} & + \text{Pyrope} + \text{Diopsode} + \text{Forsterite} & \Rightarrow & \text{MgO} + \text{Mg}_2\text{Al}_2\text{Si}_2\text{O}_6 + \text{CaMgSi}_2\text{O}_4 + \text{Mg}_2\text{Si}_2\text{O}_4
\end{align*}
\]

\[
\begin{align*}
\text{Spinel} & + \text{Pyrope} + \text{Diopsode} + \text{Forsterite} & \Rightarrow & \text{Mg}_2\text{Al}_2\text{Si}_2\text{O}_6 + \text{CaMgSi}_2\text{O}_4 + \text{Mg}_2\text{Si}_2\text{O}_4
\end{align*}
\]

\[
\begin{align*}
\text{Monticellite} & + \text{Pyrope} + \text{Diopsode} + \text{Forsterite} & \Rightarrow & \text{Mg}_2\text{CaSi}_2\text{O}_4 + \text{Mg}_3\text{Al}_2\text{Si}_2\text{O}_6 + \text{CaMgSi}_2\text{O}_4 + \text{Mg}_2\text{Si}_2\text{O}_4
\end{align*}
\]

should define a invariant point in $P-T$ space. The position of this point is unknown and should have a significant effect upon models of low-silica petrogenetic systems.
There are several possible improvements in the norm algorithm. The assumption of K-bearing pyroxenes can result in highly unlikely pyroxene compositions if the rock contains more than 1 percent K2O. Sanidine perhaps is a more reasonable phase for higher K compositions. Sanidine is stable to at least 1200°C and 40 kbar (Lindsley, 1966), and has been observed as a primary phase in an eclogite inclusion in kimeterite (Smyth and Hatton, 1977). However, it has never been observed as a primary phase in a mantle-derived peridotite.

The program does not allow Ca to enter garnet unless there is a large excess of Ca over Mg + Fe2+, in which case no Mg or Fe enters the garnet. Some appropriate partitioning factors for allowing Ca to enter pyrope-almandine garnet would approach more closely observed mineral compositions. Also, nonstoichiometric pyroxenes (Smyth, 1980) are abundant in natural samples, but are not considered here.

For geophysical modeling of mantle densities, the effects of pressure and temperature on density should be considered. Although, to a first approximation, the two effects nearly cancel each other so that STP densities should not deviate from densities at 30 kbar and 1000°C by more than 1 or 2 percent, the effects may become important if large temperature variations are considered. Thermal expansions (at one atmosphere) and compressibilities (usually at 20°C) are fairly well known for most of these phases, but measurements of thermal expansions at pressure and compressibilities at high temperatures are not usual. Therefore, corrections of density for P and T are not rigorously possible, although a better estimate than STP density should be possible and may be desirable.

CONCLUSIONS

The FORTRAN IV code, MANTLE, is a first step toward calculation of a standard sequence of mineral assemblages expected at 30 kbar pressure and prediction of their physical properties. Many improvements in the program are possible and desirable. The program has proven useful in modeling of petrogenetic processes in the terrestrial planets, and in calculation of STP densities of various bulk compositions. Use of the program has pointed up the need for some additional investigations in experimental petrology. It is hoped that publication of the code will lead to valuable use, criticism, and improvement of the program.

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REFERENCES


OTHER REFERENCES


C-----START NEW CYCLE; ZERO ARRAYS
2 DO 4 N=1,9
4 EN(N)=0.0
C-----INPUT
10 FORMAT (’ ’PROGROR TO CALCULATE MANTLE NORM,’/’ ENTER TITLE!’
READ (5,12) TITLE
12 FORMAT (8A4)
WRITE (7,14)
14 FORMAT (’ ENTER WEIGHT PERCENT OXIDES IN THE FOLLOWING ORDER:’,
1/’ SI02, AL2O3, TI02, MG0, Fe0, Fe2O3, CA0, NA2O, K2O’)
DO 20 N=1,9
WRITE (7,16)N
20 CONTINUE
IF(TOT.LE.110.0.AND.TOT.GE.90.0) GO TO 28
WRITE (7,22)
22 FORMAT (’ ANALYSIS DOES NOT TOTAL NEAR 100, TRY AGAIN!’)
GO TO 2
C-----CONVERT TO CATION NUMBERS PER 24 OXYGENS
2B DO 30 I=1,9
30 EN(I)=EN(I)/EW(I)
OXN=2.0*EN(1)+3.0*EN(2)+2.0*EN(3)+EN(4)+EN(5)+3.0*EN(6)+EN(7)
1 EN(9)=EN(9)
OX=24.0/OXN
DO 40 J=1,9
40 EN(J)=EN(J)*OX
EN(2)=2.0*EN(2)
EN(6)=2.0*EN(6)
EN(9)=2.0*EN(9)
C-----REMOVAL OF ILMENITE
IF(EN(3).GT.EN(5)) GO TO 50
EN(3)=0.0
EN(5)=EN(5)-AMN(1)
GO TO 60
C-----REMOVAL OF RUTILE
50 AMN(2)=EN(3)
EN(3)=0.0
C-----REMOVAL OF K AL SI2 O6 AMN(3)
60 AMN(3)=EN(9)
EN(9)=0.0
EN(2)=EN(2)-AMN(3)
EN(1)=EN(1)-2.0*AMN(3)
IF(EN(2).LT.0.0.OR.EN(1).LT.0.0) GO TO 500
C-----ESTABLISHMENT OF X AND Y RATIOS
X=EN(4)/EN(5)
XR=EN(4)/X
Y=EN(2)/EN(6)
YR=EN(2)/Y
WRITE(7,62)X,Y,XR,YR
C-----REMOVAL OF JADEITE
IF(Y.LT.EN(8)) GOTO 500
AMN(4)=Y*EN(8)
EN(8)=EN(8)-AMN(4)
EN(2)=EN(2)-AMN(4)
EN(1)=EN(1)-2.0*AMN(4)
IF(EN(1).LT.0.0) GO TO 500
C-----REMOVAL OF ACHLITE NA FE SI2 O6 AMN(5)
AMN(5)=EN(8)
EN(8)=0.0
EN(6)=EN(6)-AMN(5)
EN(1)=EN(1)-2.0*AMN(5)
IF(EN(1).LT.0.0) GO TO 500
C-----REMOVAL OF ANDRADITE CA3 FE2 SI3 O12 AMN(6)
AMN(6)=EN(6)/2.0
IF(EN(6)/2.0.GT.EN(1)/3.0.OR.EN(6)/2.0.GT.EN(7)/3.0) GO TO 502
EN(6)=0.0
EN(7)=EN(7)-3.0*AMN(6)
EN(1)=EN(1)-3.0*AMN(6)
C-----SPLIT ON CALCIUM
IF(EN(7).GT.X) GO TO 300
C-----REMOVAL OF DIOPSIDE CA MO SI2 O6 AMN(7)
AMN(7)=EN(7)*XR
EN(7)=EN(7)-AMN(7)
EN(4)=EN(4)-AMN(7)
EN(1)=EN(1)-2.0*AMN(7)
C-----REMOVAL OF HEDEWBERGITE CA FE SI2 O6 AMN(8)
AMN(8)=EN(7)
EN(7)=0.0
EN(5)=EN(5)-AMN(8)
EN(1)=EN(1)-2.0*AMN(7)
IF(EN(1).LT.0.0) GO TO 504
BRANCH FOR EXCESS AL
IF((EN(4)<EN(5))/3.0).LT.(EN(2)/2.0)) GO TO 200

BRANCH OUT FOR SILICA DEFICIENT
IF((EN(2)/2.0).LT.(EN(1)/3.0)) GOTO 100

REMOVAL OF PYROPE MG3 AL2 SI3 O12 AMN(10)
AMN(10)=XREW(2)/2.0
EN(4)=EN(4)-3.0*AMN(10)
EN(2)=EN(2)-2.0*AMN(10)
EN(1)=EN(1)-3.0*AMN(10)

REMOVAL OF ALMANDINE FE3 AL2 SI3 O12 AMN(11)
AMN(11)=EN(2)
EN(2)=0.0
EN(5)=EN(5)-3.0*AMN(11)
EN(1)=EN(1)-3.0*AMN(11)

CALCULATE SIX RATIO AND BRANCH
SIX=EN(1)/(EN(4)+EN(5))
WRITE(7,70) SIX
70 FORMAT(' SIX = ',F8.4)
IF(SIX.LT.0.5) GO TO 90
IF(SIX.LT.1.0) GO TO 80

EXCESS SILICA (SIX.GT.1)

REMOVAL OF ENSTATITE MG2 SI2 O6 AMN(14)
AMN(14)=EN(4)/2.0
EN(4)=0.0
EN(1)=EN(1)-2.0*AMN(14)

REMOVAL OF FORSTERITE
AMN(15)=EN(5)/2.0
EN(5)=0.0
EN(1)=EN(1)-2.0*AMN(15)

REMOVAL OF COESITE SI O2 AMN(22)
AMN(22)=EN(1)
EN(1)=0.0
GO TO 400

1.GT.SIX.GT.1/2

REMOVAL OF ENSTATITE MG2 SI2 O6 AMN(14)
80 AMN(14)=XREW(1)-((EN(4)+EN(5))/2.0))
EN(4)=EN(4)-2.0*AMN(14)
EN(1)=EN(1)-2.0*AMN(14)

REMOVAL OF FORSTERITE FE2 SI2 O6 AMN(15)
AMN(15)=(1.0-XR)*AMN(14)/XR
EN(5)=EN(5)-AMN(15)/2.0
EN(1)=EN(1)-2.0*AMN(15)

REMOVAL OF FORSTERITE MG2 SI O4 AMN(17)
AMN(17)=EN(1)
EN(1)=EN(1)-AMN(17)
EN(4)=EN(4)-2.0*AMN(17)
IF(EN(4).LT.-0.02.OR.EN(4).GT.0.02)WRITE(7,81)
81 FORMAT(' ERROR IN THE REMOVAL OF FORSTERITE')

REMOVAL OF FAYALITE FE2 SI O4 AMN(18)
AMN(18)=EN(1)
EN(1)=0.0
EN(5)=EN(5)-2.0*AMN(18)
GOTO 400

SIX<1/2: EXCESS X

REMOVAL OF FORSTERITE MG2 SI O6 AMN(17)
90 AMN(17)=XREW(1)
EN(4)=EN(4)-2.0*AMN(17)
EN(1)=EN(1)-AMN(17)

REMOVAL OF FAYALITE FE2 SI O6 AMN(18)
AMN(18)=EN(1)
EN(1)=0.0
EN(5)=EN(5)-2.0*AMN(18)

REMOVAL OF PERICLASE MG O AMN(24)
95 AMN(24)=EN(4)
EN(4)=0.0

REMOVAL OF WUSTITE FE O AMN(23)
AMN(23)=EN(5)
EN(5)=0.0
GOTO 400

GARNET SILICA LIMITED (X/3+Y/2)+(Y/2+Z/3)

REMOVAL OF PYROPE MG3 AL2 SI3 O12 AMN(10)
100 AMN(10)=XREW(1)/3.0
EN(1)=EN(1)-3.0*AMN(10)
EN(2)=EN(2)-2.0*AMN(10)
EN(4)=EN(4)-3.0*AMN(10)

REMOVAL OF ALMANDINE FE3 AL2 SI3 O12 AMN(11)
AMN(11)=EN(1)/3.0
EN(1)=0.0
EN(2)=EN(2)-2.0*AMN(11)
EN(5)=EN(5)-3.0*AMN(11)

BRANCH TO 150 IF X LIMITED
120 IF((EN(4)+EN(5))/).LT.(EN(2)/2.0)GOTO 150

REMOVAL OF SPINELS (AL-LIMITED)

REMOVAL OF SPINEL MG AL2 O4 AMN(12)
AMN(12)=XREW(2)/2.0
EN(2)=EN(2)-2.0*AMN(12)
EN(4)=EN(4)-AMN(12)

REMOVAL OF MERCYRITE FE AL2 O4 AMN(13)
AMN(13)=EN(2)/2.0
EN(2)=0.0
EN(5)=EN(5)-AMN(13)
GO TO 95

REMOVAL OF SPINELS (X-LIMITED)

REMOVAL OF SPINEL MG AL2 O4 AMN(12)
150 ANN(12)=EN(4)
EN(4)=0.0
EN(2)=EN(2)-2.0*ANN(12)

C-----REMOVAL OF HEDENBERGITE (X-LIMITED) FE AL2 O4 ANN(13)
ANN(13)=EN(5)
EN(5)=0.0
EN(2)=EN(2)-2.0*ANN(13)

C-----REMOVAL OF CORUNDUM AL2 O3 AMN(21)
ANN(21)=EN(2)/2.0
EN(2)=0.0
GO TO 400

C-----BRANCH FOR Y/2>X/3 EXCESS AL
C-----BRANCH TO 250 IF SILICA LIMITED
200 IF((EN(4)+EN(5))..GT.EN(1)) GO TO 250

C-----REMOVAL OF PYROPE WHEN X LIMITED MG3 AL2 SI3 O12 ANN(10)
ANN(10)=EN(4)/3.0
EN(4)=0.0
EN(1)=EN(1)-3.0*ANN(10)
EN(2)=EN(2)-2.0*ANN(10)

C-----REMOVAL OF ALMANDINE FE3 AL2 SI3 O12 ANN(11)
ANN(11)=EN(5)/3.0
EN(5)=0.0
EN(1)=EN(1)-3.0*ANN(11)
EN(2)=EN(2)-2.0*ANN(11)

C-----AL/2 > SI
210 IF(EN(2)/2.0.LT.EN(1)) GO TO 220

C-----REMOVAL OF KYANITE (SILICA LIMITED) AL2 SI O5 ANN(20)
ANN(20)=EN(1)
EN(1)=0.0
EN(2)=EN(2)-2.0*ANN(20)

C-----REMOVAL OF CORUNDUM AL2 O3 AMN(21)
ANN(21)=EN(2)
EN(2)=0.0
GO TO 400

C-----REMOVAL OF KYANITE (ALUMINA LIMITED) AL2 SI O5 ANN(20)
220 ANN(20)=EN(2)/2.0
EN(2)=0.0
EN(1)=EN(1)-ANN(20)

C-----REMOVAL OF COESITE AMN(22)=EN(1)
EN(1)=0.0
GO TO 400

C-----REMOVAL OF PYROPE (SILICA LIMITED) MG3 AL2 SI3 O12 ANN(10)
250 ANN(10)=XRE*EN(1)/3.0
EN(1)=EN(1)-3.0*ANN(10)
EN(2)=EN(2)-2.0*ANN(10)
EN(4)=EN(4)-3.0*ANN(10)

C-----REMOVAL OF ALMANDINE (SILICA LIMITED) FE3 AL2 SI3 O12 ANN(11)
ANN(11)=EN(1)/3.0
EN(1)=0.0
EN(2)=EN(2)-2.0*ANN(11)
EN(5)=EN(5)-3.0*ANN(11)
GO TO 120

C***********************************************************************************************

C-----CA IN EXCESS OF X
C-----REMOVAL OF DIOPSIDE (X-LIMITED) CA MG SI2 O6 ANN(7)
300 ANN(7)=EN(4)
EN(4)=0.0
EN(1)=EN(1)-2.0*ANN(7)
EN(7)=EN(7)-ANN(7)

C-----REMOVAL OF HEDENBERGITE (X-LIMITED) CA FE SI2 O6
ANN(8)=EN(5)
EN(5)=0.0
EN(1)=EN(1)-2.0*ANN(8)
EN(7)=EN(7)-ANN(8)

C-----BRANCH TO 350 FOR CA/3<AL/2
C-----BRANCH TO 330 FOR INSUFFICIENT SILICA
C-----BRANCH TO 310 FOR WOLLASTONITE
C-----BRANCH TO 300 FOR ALAMANDINE
C-----BRANCH TO 250 FOR PYROPE

C-----REMOVAL OF GROSULAR (AL-LIMITED) CA3 AL2 SI3 O12 ANN(9)
ANN(9)=EN(2)/2.0
EN(1)=EN(1)-3.0*ANN(9)
EN(2)=0.0
EN(7)=EN(7)-3.0*ANN(9)

C-----BRANCH TO 310 FOR WOLLASTONITE
C-----BRANCH TO 300 FOR ALAMANDINE
C-----BRANCH TO 250 FOR PYROPE

C-----REMOVAL OF MONTICELLIITE CA2 SI O4 ANN(19) SILICA LIMITED
ANN(19)=EN(1)
EN(1)=0.0
EN(7)=EN(7)-2.0*ANN(19)

C-----REMOVAL OF CALCIA CA O ANN(25)
ANN(25)=EN(7)
EN(7)=0.0
GO TO 400

C-----REMOVAL OF WOLLASTONITE/MONTICELLIITE
C-----BRANCH FOR SILICA EXCESS
310 IF(EN(7).LT.EN(1)) GO TO 320

C-----REMOVAL OF WOLLASTONITE CA2 SI O6 ANN(16)
ANN(16)=EN(1)+EN(7)/2.0
EN(1)=EN(1)-2.0*ANN(16)
EN(7)=EN(7)-2.0*ANN(16)

C-----REMOVAL OF MONTICELLIITE CA2 SI O4 ANN(19)
ANN(19)=EN(1)
EN(1)=0.0
EN(7)=0.0
GO TO 400

C-------REMOVAL OF WOLLASTONITE (CA-LIMITED)    CA251206    AMN(16)
320    AMN(16)=EN(7)/2.0
EN(7)=0.0
EN(1)=EN(1)-2.0*AMN(16)

C-------REMOVAL OF COESITE    SI 02    AMN(22)
AMN(22)=EN(1)
EN(1)=0.0
GO TO 400

C

C-------REMOVAL OF GROSBULAR (SILICA LIMITED) (CA/3>AL/2) CA3 AL2 SI3 012
330    AMN(9)=EN(1)/3.0
EN(7)=EN(7)-3.0*AMN(9)
EN(1)=EN(1)-3.0*AMN(9)
EN(2)=EN(2)-3.0*AMN(9)

C-------REMOVAL OF CORUNDUM AL2 03    AMN(21)
AMN(21)=EN(2)/2.0
EN(2)=0.0

C-------REMOVAL OF CALCIA    CA 0    AMN(25)
AMN(25)=EN(7)
EN(7)=0.0
GO TO 400

C

C-------BACK TO 330 IF SILICA LIMITED
350 IF(EN(7)>GT.EN(1))GO TO 330

C-------REMOVAL OF GROSBULAR (CA-LIMITED)    CA3 AL2 SI3 012    AMN(9)
AMN(9)=EN(7)/3.0
EN(7)=0.0
EN(1)=EN(1)-3.0*AMN(9)
EN(2)=EN(2)-3.0*AMN(9)

C-------RETURN TO 210 FOR REMOVAL OF KYANITE, CORUNDUM AND COESITE
GO TO 210

C*******************************************************************************

C

C-------Calculation of mineral weight percents
400 TOTW=0.0
TOTV=0.0
TOTM=0.0
DG 410 N=1.25
AMW(N)=AMN(N)*AMAV(N)
TOTM=TOTW+AMN(N)
410 TOTV=TOTW+AMV(N)
DG 420 N=1.25
AMN(N)=AMN(N)/TOTM
420 AMW(N)=100.*AMV(N)/TOTW

C-------calculate partial volumes and density
DG 430 N=1.25
VOL(N)=AMV(N)/AMD(N)
430 TOTV=TOTV+VOL(N)
RHO=100.0/TOTV
GO TO 600

C*******************************************************************************

C

C-------ERROR MESSAGES
500 WRITE (7,501)
501 FORMAT ("THIS ROCK IS TOO ALKALIC TO BE IN THE MANTLE")
GO TO 520
502 WRITE (7,503)
503 FORMAT ("THIS ROCK HAS TOO MUCH Fe 3+ TO BE IN THE MANTLE")
GO TO 520
504 WRITE (7,505)
505 FORMAT ("RAN OUT OF SILICA IN THE REMOVAL OF DIOPSIDE/HEDEN")
520 WRITE (7,521) (EN(N),N=1,9)
521 FORMAT ("RESIDUAL ELEMENT NUMBERS: /5F8.4, /4F8.4")
GO TO 450

C*******************************************************************************

C

C-------OUTPUT
600 WRITE (7,602) TITLE
602 FORMAT ("///",18A4)
DG 620 N=1.25
IF(AMW(N).LT.0.00001.AND.AMW(N).GT.-0.00001) GO TO 620
NO=N-1
N1=3*N0+1
N2=3*N0+2
N3=3*N0+3
WRITE (7,610)TMN(N1),TMN(N2),TMN(N3),AMW(N)
610 FORMAT (3A4,3X,F8.4)
620 CONTINUE
WRITE (7,630) RHO
630 FORMAT ("THE DENSITY OF THIS ROCK IS F8.4")
650 WRITE (7,652)
652 FORMAT ("TYPE 0 TO END, 1 FOR ANOTHER CYCLE;")
READ (5,654) L
654 FORMAT (I1)
IF(L.EQ.1) GO TO 2
CALL EXIT
END