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N65-30456

FACILITY FORM 602

(ACCESSION NUMBER)	(THRU)
20 (PAGES)	1 (CODE)
CR 64200 (NASA CR OR TMX OR AD NUMBER)	06 (CATEGORY)

GPO PRICE $ _____

CFSTI PRICE(S) $ _____

Hard copy (HC) _____

Microfiche (MF) _____

ff 653 July 65

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IBM FORTRAN PROGRAM FOR THE CALCULATION OF CIPW IGNEOUS ROCK NORMS

IBM FORTRAN PROGRAM FOR THE CALCULATION OF CIPW IGNEOUS ROCK NORMS

by

Peter Deines

Technical Report.

Prepared under Contract No. NASW-1062

by

Nuclide Corporation
State College, Pennsylvania

for

National Aeronautics and Space Administration

Nuclide T. R. 65-09 1 June 1965

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INTRODUCTION

An IBM FULL FORTRAN computer program has been designed to calculate the normative composition of igneous rocks ("igneous rock norms") from chemical analyses containing up to 23 elements. It uses the method given by Johannsen(1) and first proposed by Cross, Iddings, Pirsson, and Washington (2). The print-out of the program comprises:

1. Self-explanatory headings and sample identification,

2. a list of the oxides used in the computation, and the sum of these oxides,

3. the weight percent of the 12 salic and 19 femic normative minerals (listed in Figure 3) and the sum of the salic and the sum of the femic minerals, and

4. the molecular ratio of MgO/FeO, in hypersthene, diopside and olivine, as calculated.

Carbon dioxide appearing in a given chemical analysis may be recalculated either as sodium carbonate or as calcite, but not both simultaneously,at the option of the user.

INPUT

One parameter card and three cards for the analytical data contain all the information required to make a rock norm calculation for one sample.

Parameter Card

Columns 1 to 10 - Sample identification. These columns may contain alphabetic characters, numerical digits, special characters permitted by processor, and up to 9 blank spaces or zeros. Ten zeros or blanks in this field signify end-of-file and stop the program.

Columns 11 to 13 - Calculation of CO_2 as sodium carbonate.
Punch +1, CO_2 is recalculated as sodium carbonate.
Punch 00, no sodium carbonate is calculated.

Columns 14 to 16 - Calculation of CO_2 as calcium carbonate.
Punch +1, CO_2 is recalculated as calcium carbonate.
Punch 00, no calcium carbonate is calculated.

It is not possible to calculate sodium carbonate and calcite simultaneously with this program; hence, one of the two sets of columns has always to be zero. If CO_2 is present in the analysis but one does not wish to calculate Na_2CO_3 or $CaCO_3$ he may set both sets to contain blanks; in this case the program ignores the CO_2.

Data Cards

The weight percentages of the oxides and elements listed in the analysis to be recalculated as a rock norm are punched on three data cards in floating point notation (decimal points must be punched).

Data card 1: Ten columns for each oxide in the following sequence: SiO_2, Al_2O_3, Fe_2O_3, FeO, MgO, CaO, Na_2O, K_2O.

Data card 2: Ten columns for each oxide and element in the following sequence: TiO_2, P_2O_5, MnO, ZrO, CO_2, SO_3, Cl_2, F_2

Data card 3: Ten columns for each element and oxide in the following sequence: S, Cr_2O_3, NiO, CoO, BaO, SrO, Li_2O

If analytical data are not available for certain elements, 0.0 should be entered in the appropriate field.

There is no limit to the number of rock norms which may be calculated in one run or execution of the program. A parameter card precedes each set of 3 data cards, and a blank card at the end of the input deck will terminate the calculation procedure.

PROGRAM TESTING

A flow chart indicating the logical circuits, i.e. the sequence of computation for all possible conditions, is shown in Figure 1. The FORTRAN program is given in Figure 2. Wherever possible, standard chemical symbols and mineralogical abbreviations have been used. If the standard abbreviation begins with a letter I to N reserved by FORTRAN for fixed point variables, the

abbreviation is prefixed by A to make floating point calculation possible. An example of the print-out provided by the program is shown in Figure 3.

The program was tested with 50 rock analyses, covering a wide range of chemical and mineralogical compositions, taken from Clarke (3). The IBM 7074 Computer in The Pennsylvania State University Computation Center was used. Norms produced by this program were found to be in close agreement with those of Clarke except in cases where discrepancies were traced to errors in Clarke's computation or were shown to arise from differences in the type of norm calculation used. The execute time for calculation of one chemical analysis was 2 sec.

ACKNOWLEDGEMENTS

This work was made possible by the National Aeronautics and Space Agency under Contract NASW-1062 and by the Computation Center of The Pennsylvania State University which provided support for the computer time. This support is gratefully acknowledged. The helpful suggestions of Dr. L. F. Herzog are also appreciated.

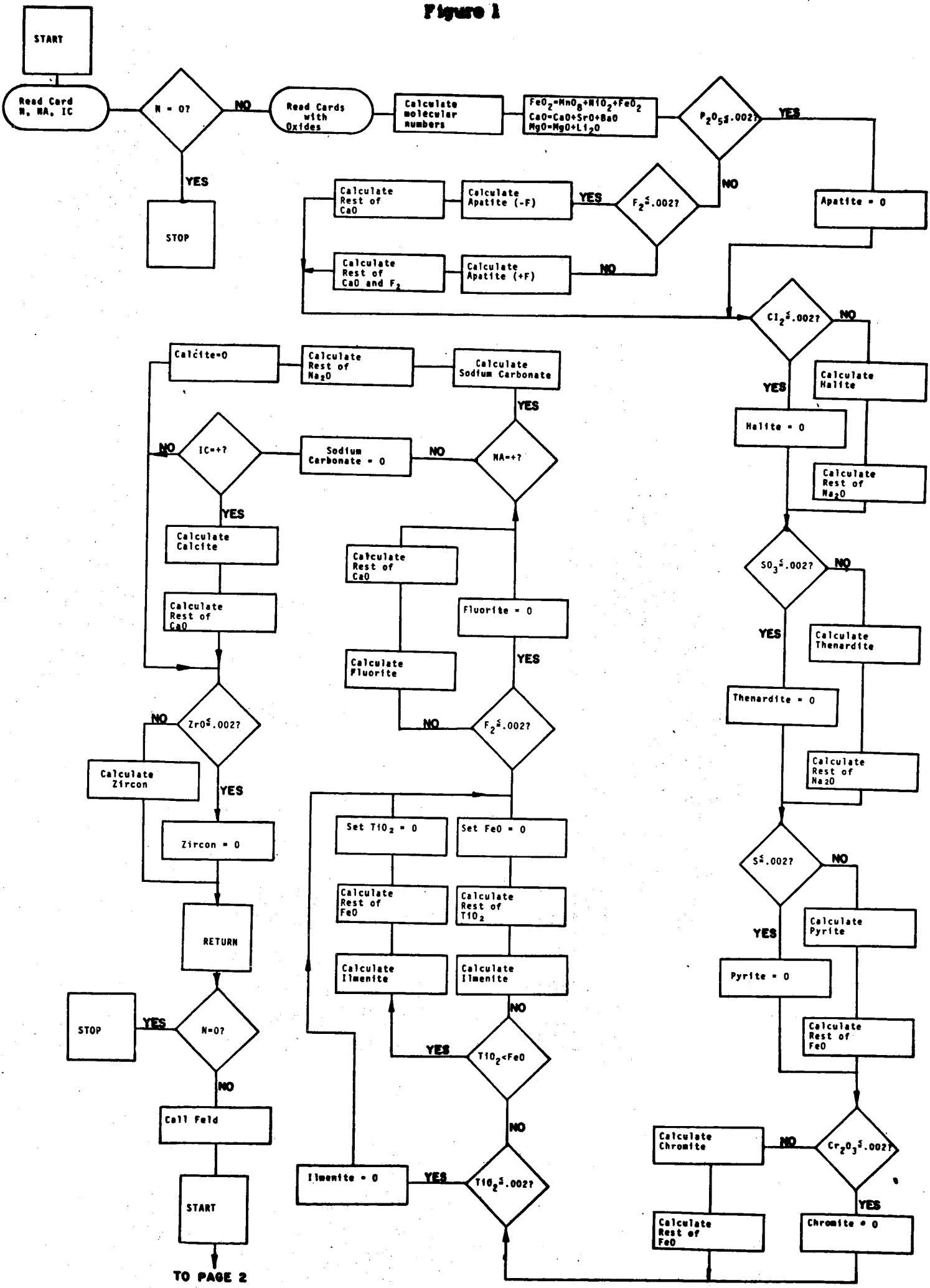
REFERENCES

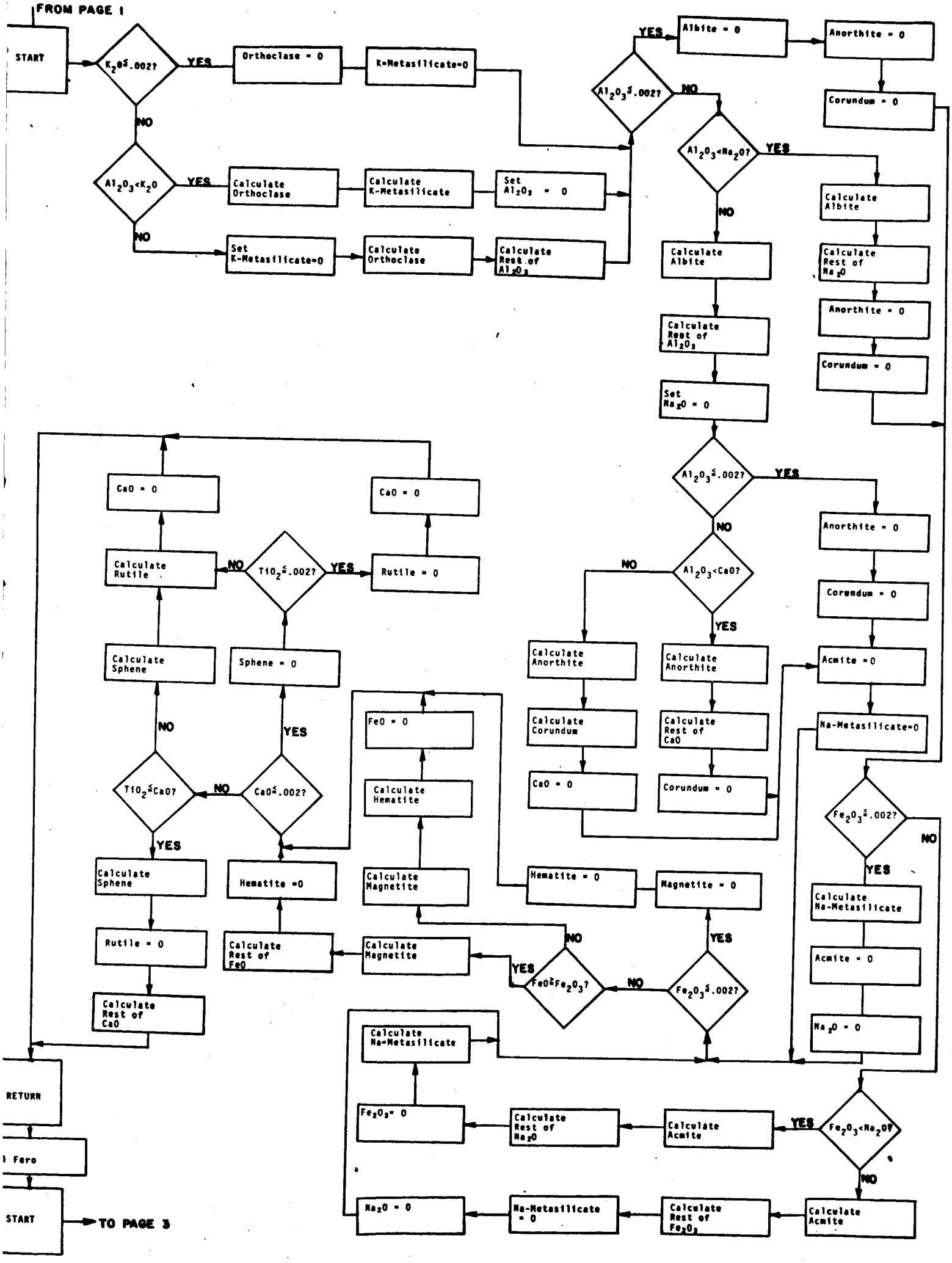
1. Johannsen, A., Manual of Petrographic Methods, 2nd Ed., McGraw Hill (1918).

2. Washington, H. S., Chemical Analysis of Igneous Rocks, U.S. Geol. Survey Prof. Paper 99, p. 1162 (1917).

3. Clarke, F. W., The Data of Geochemistry, Geol. Survey Bull. 770, 841 pp (1924).

Figure 1


START
Read Card N, NA, IC
N = 0?
NO
YES
STOP
Read Cards with Oxides
Calculate molecular numbers
FeO2=MnO8+MnO2+FeO2
CaO=CaO+SrO+BaO
MgO=MgO+Li2O
P2O5≤.002?
YES
NO
Apatite = 0
Calculate Rest of CaO
Calculate Apatite (-F)
F2≤.002?
YES
NO
Calculate Rest of CaO and F2
Calculate Apatite (+F)
Cl2≤.002?
NO
YES
Calculate Halite
Halite = 0
Calculate Rest of Na2O
SO3≤.002?
NO
YES
Calculate Thenardite
Thenardite = 0
Calculate Rest of Na2O
S≤.002?
NO
YES
Calculate Pyrite
Pyrite = 0
Calculate Rest of FeO
Cr2O3≤.002?
YES
Chromite = 0
Calculate Chromite
NO
Calculate Rest of FeO
Calcite=0
Calculate Rest of Na2O
Calculate Sodium Carbonate
YES
NA=+?
NO
Sodium Carbonate = 0
NO
IC=+?
YES
Calculate Calcite
Calculate Rest of CaO
ZrO≤.002?
NO
YES
Calculate Zircon
Zircon = 0
RETURN
N=0?
YES
STOP
NO
Call Feld
START
TO PAGE 2
Calculate Rest of CaO
Fluorite = 0
Calculate Fluorite
F2≤.002?
NO
YES
Set TiO2 = 0
Set FeO = 0
Calculate Rest of FeO
Calculate Rest of TiO2
Calculate Ilmenite
Calculate Ilmenite
TiO2<FeO
YES
NO
TiO2≤.002?
YES
Ilmenite = 0
NO


FROM PAGE 1
START
$K_2O \leq .002$?
YES
Orthoclase = 0
K-Metasilicate=0
NO
$Al_2O_3 < K_2O$
YES
Calculate Orthoclase
Calculate K-Metasilicate
Set Al_2O_3 = 0
NO
Set K-Metasilicate=0
Calculate Orthoclase
Calculate Rest of Al_2O_3
$Al_2O_3 \leq .002$?
YES
Albite = 0
Anorthite = 0
Corundum = 0
NO
$Al_2O_3 < Na_2O$?
YES
Calculate Albite
Calculate Rest of Na_2O
Anorthite = 0
Corundum = 0
NO
Calculate Albite
Calculate Rest of Al_2O_3
Set Na_2O = 0
$Al_2O_3 \leq .002$?
YES
Anorthite = 0
Corundum = 0
Acmite = 0
Na-Metasilicate=0
NO
$Al_2O_3 < CaO$?
NO
Calculate Anorthite
Calculate Corundum
CaO = 0
YES
Calculate Anorthite
Calculate Rest of CaO
Corundum = 0
CaO = 0
$TiO_2 \leq .002$?
YES
Rutile = 0
NO
Calculate Rutile
CaO = 0
Calculate Sphene
Sphene = 0
NO
$TiO_2 \leq CaO$?
YES
Calculate Sphene
Rutile = 0
Calculate Rest of CaO
NO
$CaO \leq .002$?
YES
Hematite =0
Calculate Rest of FeO
Calculate Magnetite
FeO = 0
Calculate Hematite
Calculate Magnetite
Hematite = 0
Magnetite = 0
NO
$FeO \geq Fe_2O_3$?
YES
NO
$Fe_2O_3 \leq .002$?
YES
$Fe_2O_3 \leq .002$?
NO
YES
Calculate Na-Metasilicate
Acmite = 0
Na_2O = 0
Calculate Na-Metasilicate
Fe_2O_3 = 0
Calculate Rest of Na_2O
Calculate Acmite
YES
$Fe_2O_3 < Na_2O$?
NO
Na_2O = 0
Na-Metasilicate = 0
Calculate Rest of Fe_2O_3
Calculate Acmite
RETURN
Fero
START
TO PAGE 3

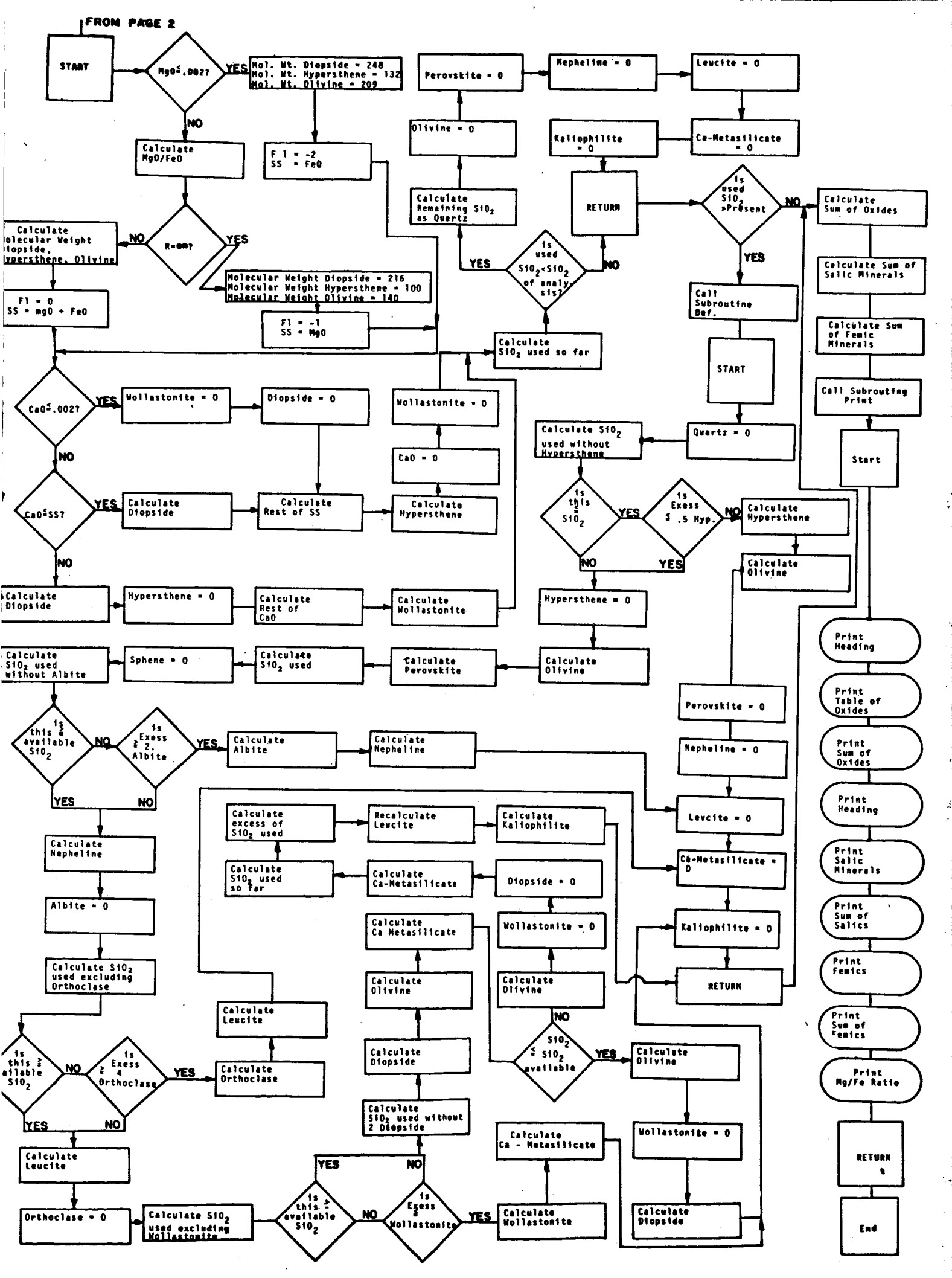

FROM PAGE 2
START
MgO≤.002?
YES
NO
Mol. Wt. Diopside = 248
Mol. Wt. Hypersthene = 132
Mol. Wt. Olivine = 209
Calculate MgO/FeO
F 1 = -2
SS = FeO
R=∞?
Calculate Molecular Weight Diopside, Hypersthene, Olivine
Molecular Weight Diopside = 216
Molecular Weight Hypersthene = 100
Molecular Weight Olivine = 140
F1 = 0
SS = mgO + FeO
F1 = -1
SS = MgO
CaO≤.002?
Wollastonite = 0
Diopside = 0
CaO≤SS?
Calculate Diopside
Calculate Rest of SS
Calculate Hypersthene
Calculate Diopside
Hypersthene = 0
Calculate Rest of CaO
Calculate Wollastonite
Wollastonite = 0
CaO = 0
Calculate Sphene = 0
Calculate SiO2 used without Albite
Is this ≥ available SiO2
Is Excess ≥ 2. Albite
Calculate Albite
Calculate Nepheline
Calculate Nepheline
Albite = 0
Calculate SiO2 used excluding Orthoclase
Is this ≥ available SiO2
Is Excess ≥ 4 Orthoclase
Calculate Orthoclase
Calculate Leucite
Calculate Leucite
Orthoclase = 0
Calculate SiO2 used excluding Wollastonite
Is this ≥ available SiO2
Is Excess ≥ Wollastonite
Calculate Wollastonite
Calculate Ca - Metasilicate
Wollastonite = 0
Calculate Diopside
Calculate SiO2 used without 2 Diopside
Calculate Diopside
Calculate Olivine
Calculate Ca Metasilicate
Calculate Olivine
Wollastonite = 0
SiO2 ≤ SiO2 available
Calculate Olivine
Calculate Hypersthene
Calculate Olivine
Hypersthene = 0
Calculate Perovskite
Calculate SiO2 used
Calculate SiO2 used without Hypersthene
Is this ≤ SiO2
Is Excess ≤ .5 Hyp.
Quartz = 0
Calculate Perovskite
Calculate Nepheline
Calculate Leucite
Calculate Ca-Metasilicate = 0
Calculate Kaliophilite = 0
RETURN
Perovskite = 0
Olivine = 0
Calculate Remaining SiO2 as Quartz
Is used SiO2<SiO2 of analysis?
Calculate SiO2 used so far
Nepheline = 0
Kaliophilite = 0
RETURN
Leucite = 0
Ca-Metasilicate = 0
Is used SiO2 Present
Call Subroutine Def.
START
Calculate Sum of Oxides
Calculate Sum of Salic Minerals
Calculate Sum of Femic Minerals
Call Subrouting Print
Start
Print Heading
Print Table of Oxides
Print Sum of Oxides
Print Heading
Print Salic Minerals
Print Sum of Salics
Print Femics
Print Sum of Femics
Print Mg/Fe Ratio
RETURN
End

Figure 2

```
      C OMPILE    RUN  FORTRAN
C     .
        CIPW NORM CACULATION MAIN PROGRAM
        DIMENSION N(2)
        COMMON N,NA,IC,SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO,AMNO,ZRO
       1 ,CO,CL,F,S,CRO,ANIO,COO,SRO,ALIO,SIO1,ALO1,FEO31,FEO21,AMGO1,CAO1,
       2 ANAO1,AKC1,TIO1,PO1,AMNO1,ZRO1,CO1,SO1,CL1,F1,S1,CRO1,ANIO1,COO1,
       3 SRO1,ALIO1,AP,HL,TH,PR,CM,AIL,FR,ANC,CC,Z,OR,AKS,AB,AN,C,AC,ANS,AM
       4 T,HM,SP,RU,R,SS,SS1,HY,AMWOI,AMWHY,AMWOL,WO,DI,OL,SIOC,PF,ANE,AB1,
       5 OR1,CS,DI1,OL1,ALC,SALG,FEMG,ALC1,SO,SIOC1,BAO,BAO1,AKP,Q,SUM
     1   CALL ACCESS
         IF (N(2)) 2222,2222,2
     2   CALL FELD
         CALL FERO
         IF(SIO1-SIOC1)73,1118,1118
    73   CALL DEF
  1118   SUM = SIO+ALO+FEO3+AMGO+CAO+ANAO+AKO+TIO+PO+AMNO+ZRO+CO+SO+
       1 CL+F+CRO+ANIO+COO+BAO+SRO+ALIO +S+FEO2
         SALG = Q+C+Z+OR+AB+AN+ALC+ANE+AKP+HL+TH+ANC
         FEMG = AC+ANS+AKS+DI+WO+HY+OL+CS+AMT+CM+HM+AIL+SP+PF+RU+AP+FR+
       1 PR+CC
         CALL PRINT
  3333   GO TO 1
  2222   STOP
         END
```

```
      C OMPILE   RUN  FORTRAN
        SUBROUTINE ACCESS
        DIMENSION N(2)
        COMMON N,NA,IC,SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO,AMNO,ZRO
       1 ,CO,CL,F,S,CRO,ANIO,COO,SRO,ALIO,SIO1,ALO1,FEO31,FEO21,AMGO1,CAO1,
       2 ANAO1,AKO1,TIO1,PO1,AMNO1,ZRO1,CO1,SO1,CL1,F1,S1,CRO1,ANIO1,COO1,
       3 SRO1,ALIO1,AP,HL,TH,PR,CM,AIL,FR,ANC,CC,Z,OR,AKS,AB,AN,C,AC,ANS,AM
       4 T,HM,SP,RU,R,SS,SS1,HY,AMWDI,AMWHY,AMWOL,WO,DI,OL,SIOC,PF,ANE,AB1,
       5 OR1,CS,DI1,OL1,ALC,SALG,FEMG,ALC1,SO,SIOC1,BAO,BAO1,AKP,Q,SUM
        READ 1,N(1),N(2),NA,IC
    1   FORMAT ( 2A5,2I3)
        IF (N(2)) 2222,2222,2221
 2222   STOP
 2221   READ 2,SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO,AMNO,ZRO,CO,SO,C
       1 L,F,S,CRO,ANIO,COO,BAO,SRO,ALIO
    2   FORMAT (8F10.0)
         SIO1 = SIO/60.
        ALO1 = ALO/102.
        FEO31 = FEO3/160.
         FEO21 = FEO2/72.
         AMGO1 = AMGO/40.
         CAO1 = CAO/56.
        ANAO1 = ANAO/62.
        AKO1 = AKO/94.
         TIO1 = TIO/80.
         PO1 = PO/142.
         AMNO1 = AMNO/71.
         ZRO1 = ZRO/123.
         CO1 = CO/44.
         SO1 = SO/80.
         CL1 = CL/71.
         F1 = F/38.
        S1 = S/32.
        CRO1 = CRO/152.
         ANIO1 = ANIO/75.
        COO1 = COO/75.
        BAO1 = BAO/153.5
         SRO1 = SRO/103.5
        ALIO1 = ALIO/30.
         FEO21 = AMNO1 + ANIO1 + FEO21
        CAO1 = CAO1 + SRO1 + BAO1
        AMGO1 = AMGO1 + ALIO1
        IF(PO1-.002)3,3,4
    4   IF(F1-.002)141,141,142
  141   AP = PO1*310.
        CAO1 = CAO1-3.*PO1
        GO TO 5
  142   AP = PO1*336.
        CAO1 = CAO1-3.3333*PO1
        F1 = F1-.3333*PO1
        GO TO 5
    3   AP = 0.
    5   IF(CL1-.002)6,6,7
    6   HL = 0.
        GO TO 8
    7   HL = 2.*CL1*117.
        ANAO1 = ANAO1-CL1
    8   IF(SO1-.002)9,9,10
   10   TH = SO1*142.
```

```
      ANAO1 = ANAO1-SO1
      GO TO 11
    9 TH = 0.
   11 IF(S1-.002)12,12,13
   13 PR = S1*60.
      FEO21 = FEO21-.5*S1
      GO TO 14
   12  PR = 0.
   14 IF(CRO1 - .002)15,15,16
   16 CM = CRO1*224.
      FEO21 = FEO21-CRO1
      GO TO 17
   15 CM = 0.
   17 IF(TIO1-.002)18,18,19
   18 AIL = 0.
      GO TO 20
   19 IF(FEO21-TIO1)21,22,22
   21 AIL = FEO21*152.
      TIO1 = TIO1-FEO21
      FEO21 = 0.
      GO TO 20
   22 AIL = TIO1*152.
      FEO21 = FEO21-TIO1
      TIO1 = 0.
   20 IF(F1-.002)23,23,24
   23 FR = 0.
      GO TO 25
   24 FR = F1*78.
      CAO1 = CAO1-F1
   25 IF(NA)26,26,27
   27 ANC = CO1*106.
      ANAO1 = ANAO1-CO1
      CC = 0.
      GO TO 28
   26 ANC = 0.
      IF(IC)29,29,30
   30 CC = CO1*100.
      CAO1 = CAO1-CO1
      GO TO 28
   29 CC = 0.
   28 IF(ZRO1-.002)31,31,32
   31 Z = 0.
      GO TO 33
   32 Z = ZRO1*183.
   33 RETURN
      END
```

```
    C OMPILE   RUN  FORTRAN
      SUBROUTINE FERO
      DIMENSION N(2)
      COMMON N,NA,IC,SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO,AMNO,ZRO
     1 ,CO,CL,F,S,CRO,ANIO,COO,SRO,ALIO,SIO1,ALO1,FEO31,FEO21,AMGO1,CAO1,
     2 ANAO1,AKO1,TIO1,PO1,AMNO1,ZRO1,CO1,SO1,CL1,F1,S1,CRO1,ANIO1,COO1,
     3 SRO1,ALIO1,AP,HL,TH,PR,CM,FE,FR,ANC,CC,Z,OR,AKS,AB,AN,C,AC,ANS,AM
     4 T,HM,SP,RU,R,SS,SS1,HY,AMWDI,AMWHY,AMWOL,WO,DI,OL,SIOC,PF,ANE,AB1,
     5 OR1,CS,DI1,OL1,ALC,SALG,FEMG,ALC1,SO,SIOC1,BAO,BAO1,AKP,Q,SUM
  64   IF(AMGO1-.002)643,643,644
 644   R= AMGO1/FEO21
      IF DIVIDE CHECK 641,642
 641   AMWDI = 216.
      AMWHY = 100.
      AMWOL = 140.
      F1 = -1.
      SS = AMGO1
      GO TO 645
 643   AMWDI = 248.
      AMWHY = 132.
      F1 = -2.
      SS = FEO21
      AMWOL = 204.
      GO TO 645
 642   AMWDI = 56.+2.*60.+(40.*R+72.)/(R+1.)
      AMWHY = (40.*R+72.)/(R+1.)+60.
      AMWOL = 2.*(40.*R+72.)/(R+1.)+60.
      F1 = 0.
      SS = AMGO1 + FEO21
 645   IF(CAO1-.002)66,66,65
  65   IF(CAO1-SS)68,68,67
  67   DI = SS*AMWDI
      HY = 0.
      SS1 = 0.
      CAO1 = CAO1-SS
      WO = CAO1*116.
      GO TO 69
  68   DI = CAO1*AMWDI
 671   SS1 = SS-CAO1
      HY = SS1*AMWHY
      CAO1 = 0.
      WO = 0.
      GO TO 69
  66   WO = 0.
      DI = 0.
      GO TO 671
  69   SIOC = Z/183.+SP/196.+4.*AC/462.+AKS/154.+ANS/122.+6.*OR/556.+6.*A
     1 B/524.+2.*AN/278.+2.*DI/AMWDI+WO/116.+HY/AMWHY
      SIOC1 = SIOC
  71   IF(SIO1-SIOC1)73,72,72
  72   Q = (SIO1-SIOC1)*60.
      OL = 0.
      PF = 0.
      ANE = 0.
      ALC = 0.
      CS = 0.
      AKP = 0.
  73   RETURN
      END
```

```
   C OMPILE   RUN  FORTRAN
     SUBROUTINE FELD
     DIMENSION N(2)
     COMMON N,NA,IC,SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO,AMNO,ZRO
    1 ,CO,CL,F,S,CRO,ANIO,COO,SRO,ALIO,SIO1,ALO1,FEO31,FEO21,AMGO1,CAO1,
    2 ANAO1,AKO1,TIO1,PO1,AMNO1,ZRO1,CO1,SO1,CL1,F1,S1,CRO1,ANIO1,COO1,
    3 SRO1,ALIO1,AP,HL,TH,PR,CM,AIL,FR,ANC,CC,Z,OR,AKS,AB,AN,C,AC,ANS,AM
    4 T,HM,SP,RU,R,SS,SS1,HY,AMWOI,AMWHY,AMWOL,WO,DI,OL,SIOC,PF,ANE,AB1,
    5 OR1,CS,DI1,OL1,ALC,SALG,FEMG,ALC1,SO,SIOC1,BAO,BAO1,AKP,Q,SUM
 33   IF(AKO1-.002)34,34,35
 34   OR = 0.
      AKS = 0.
      GO TO 36
 35   IF(ALO1-AKO1)37,37,38
 37   OR = ALO1*556.
      AKS = (AKO1-ALO1)*154.
      ALO1 = 0.
      GO TO 36
 38   AKS = 0.
      OR = AKO1*556.
      ALO1 = ALO1-AKO1
 36   IF(ALO1-.002)39,39,40
 40   IF(ALO1-ANAO1)41,41,42
 41   AB = ALO1*524.
      ANAO1 = ANAO1-ALO1
      AN = 0.
      C = 0.
      GO TO 49
 42   AB = ANAO1*524.
      ALO1 = ALO1-ANAO1
      ANAO1 = 0.
      IF(ALO1-.002)43,43,44
 43   AN = 0.
      C = 0.
 46   AC = 0.
      ANS = 0.
      GO TO 45
 44   IF(ALO1-CAO1)47,47,48
 47   AN = ALO1*278.
      CAO1 = CAO1-ALO1
      C = 0.
      GO TO 46
 48   AN = CAO1*278.
      C = (ALO1-CAO1)*102.
      CAO1 = 0.
      GO TO 46
 39   AB = 0.
      AN = 0.
      C = 0.
 49   IF(FEO31-.002)50,50,51
 51   IF(FEO31-ANAO1)521,521,531
531   AC = ANAO1*462.
      FEO31 = FEO31-ANAO1
      ANS = 0.
      ANAO1 = 0.
      GO TO 45
521   AC = FEO31*462.
      ANAO1 = ANAO1-FEO31
      FEO31 = 0.
       ANS = ANAO1 * 122.
```

```
      GO TO 45
   50 ANS = ANAO1*122.
      AC = 0.
      ANAO1 = 0.
   45 IF(FEO31-.002)54,54,55
   54 AMT = 0.
      HM = 0.
      GO TO 56
   55 IF(FEO21-FEO31)57,58,58
   57 AMT = FEO21*232.
      HM = (FEO31-FEO21)*160.
      FEO21 = 0.
      GO TO 56
   58 AMT = FEO31*232.
      HM = 0.
      FEO21 = FEO21-FEO31
   56 IF(CAO1-.002)581,581,571
  571 IF(TIO1-CAO1)60,60,59
   59 SP = CAO1*196.
   63 RU = (TIO1-CAO1)*80.
      CAO1 = 0.
      GO TO 64
   60 SP = TIO1*196.
      RU = 0.
      CAO1 = CAO1-TIO1
      GO TO 64
  581 SP = 0.
      IF(TIO1-.002)62,62,63
   62 RU = 0.
      CAO1 = 0.
   64 RETURN
      END
```

```
      WO = 0.
      SIOC1 = Z/183.+4.*AC/462.+AKS/154.+ANS/122.+2.*AN/278.+OL/AMWOL+
     1 CS/172.+2.*ANE/284.
      SICC1 = SIO1-SIOC1
      ALC1 = ((SIOC1-2.*ALC/436.)/2.)*436.
      AKP = ((4.*ALC /436.-SIOC1)/2.)*256.
      ALC = ALC1
      GO TO 1118
1113  PF = 0.
1114  ANE = 0.
1115  ALC = 0.
1116  CS = 0.
1117  AKP = 0.
1118  RETURN
      END
```

```
   C OMPILE   RUN  FORTRAN
     SUBROUTINE DEF
     DIMENSION N(2)
     COMMON N,NA,IC,SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO,AMNO,ZRO
    1 ,CO,CL,F,S,CRO,ANIO,COO,SRO,ALIO,SIO1,ALO1,FEO31,FEO21,AMGO1,CAO1,
    2 ANAO1,AKC1,TIO1,PO1,AMNO1,ZRO1,CO1,SO1,CL1,F1,S1,CRO1,ANIO1,COO1,
    3 SRO1,ALIO1,AP,HL,TH,PR,CM,AIL,FR,ANC,CC,Z,OR,AKS,AB,AN,C,AC,ANS,AM
    4 T,HM,SP,RU,R,SS,SS1,HY,AMWDI,AMWHY,AMWOL,WO,DI,OL,SIOC,PF,ANE,AB1,
    5 OR1,CS,DI1,OL1,ALC,SALG,FEMG,ALC1,SO,SIOC1,BAO,BAO1,AKP,Q,SUM
73   Q = 0.
     SIOC1 = SIOC1-HY/AMWHY
     IF(SIO1-SIOC1)74,75,75
75   IF(SIO1-SIOC1-.5*SS1)74,74,76
76   HY1 = (2.*(SIO1-SIOC1)-SS1)*AMWHY
     OL = (SS1-HY1/AMWHY)*AMWOL/2.
     HY = HY1
     GO TO 1113
74   HY = 0.
     OL = SS1*AMWOL/2.
     PF = 136.*SP/196.
     SIOC1 = SIOC1-SP/196.
     SP = 0.
     SIOC1 = SIOC1-6.*AB/524.+OL/AMWOL
     IF(SIO1-SIOC1)77,77,78
78   IF(SIO1-SIOC1-2.*AB/524.)77,79,79
79   AB1 = ((SIO1-SIOC1-2.*AB/524.)/4.)*524.
     ANE = (AB/524.-AB1/524.) *284.
     AB = AB1
     GO TO 1115
77   ANE = (AB/524.)*284.
     AB = 0.
     SIOC1 = SIOC1-6.*OR/556.+2.*ANE/284.
     IF(SIO1-SIOC1)80,80,81
81   IF(SIO1-SIOC1-4.*OR/556.)80,82,82
82   OR1 = (SIO1-SIOC1-4.*OR/556.)/2.
     ALC = (OR/556.-OR1/556.)*436.
     OR = OR1*556.
     GO TO 1116
80   ALC = 436.*OR/556.
     OR = 0.
     SIOC1 = SIOC1-WO/116.+4.*ALC/436.
     IF(SIO1-SIOC1)83,83,841
841  IF(WO/116.-(SIO1-SIOC1))83,84,84
84   CS = (WO/116.-(SIO1-SIOC1))*172.
     WO = (WO/116.-2.*CS/172.)*116.
     GO TO 1117
83   SIOC1 = SIOC1-2.*DI/AMWDI
86   DI1 = (2.*(SIO1-SIOC1)-DI/AMWDI-(DI/AMWDI+WO/116.))/2.
     OL1 = ((DI/AMWDI-DI1)/2.)*AMWOL
     CS = (DI/AMWDI+WO/116.-DI1)/2.
     CS = CS*172.
     IF (2.*DI1      +2.*CS/172.+2.*OL1/AMWOL-2.*(SIO1-SIOC1))87,87,85
87   OL = OL+OL1
     WO = 0.
     DI = DI1*AMWDI
     GO TO 1117
85   OL = OL + AMWOL*DI/(2.*AMWDI)
     CS = 172.*DI/(2.*AMWDI) +  172.*WO/(2.*116.)
     DI = 0.
```

```
C OMPILE   RUN  FORTRAN
      SUBROUTINE PRINT
      DIMENSION N(2)
      COMMON N,NA,IC,SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO,AMNO,ZRO
     1 ,CC,CL,F,S,CRO,ANIO,COO,SRO,ALIO,SIO1,ALO1,FEO31,FEO21,AMGO1,CAO1,
     2 ANAO1,AKO1,TIO1,PO1,AMNO1,ZRO1,CO1,SO1,CL1,F1,S1,CRO1,ANIO1,COO1,
     3 SRO1,ALIO1,AP,HL,TH,PR,CM,AIL,FR,ANC,CC,Z,OR,AKS,AB,AN,C,AC,ANS,AM
     4 T,HM,SP,RU,R,SS,SS1,HY,AMWDI,AMWHY,AMWOL,WO,DI,OL,SIOC.PF,ANE,AB1,
     5 OR1,CS,DI1,OL1,ALC,SALG,FEMG,ALC1,SO,SIOC1,BAO,BAO1,AKP,Q,SUM
      PRINT 1119,N(1),N(2),SIO,ALO,FEO3,FEO2,AMGO,CAO,ANAO,AKO,TIO,PO
1119  FORMAT(1H1,52X,18HCHEMICAL ANALYSIS ,2A5/1H /1H /
     1 50X,4HSIO2,12X,F6.3/50X,5HAL2O3,11X,F6.3 /
     2 50X,5HFE2O3,11X,F6.3/50X,3HFEO,13X,F6.3/
     3 50X,3HMGO,13X,F6.3/50X,3HCAO,13X,F6.3/
     4 50X,4HNA2O,12X,F6.3/50X,3HK2O,13X,F6.3/
     5 50X,4HTIO2,12X,F6.3/50X,4HP2O5,12X,F6.3)
      PRINT 1120,AMNO,ZRO,CO,SO,CL,F,S,CRO,ANIO,COO,BAO,SRO,ALIO,SUM
1120  FORMAT(    50X,3HMNO,13X,F6.3/50X,3HZRO,13X,F6.3/
     1 50X,3HCO2,13X,F6.3/50X,3HSO3,13X,F6.3/
     2 50X,3HCL2,13X,F6.3/50X,2HF2,14X,F6.3 /
     3 50X,1HS,15X,F6.3/50X,5HCR2O3,11X,F6.3/
     4 50X,3HNIO,13X,F6.3/50X,3HCOO,13X,F6.3/ 50X,3HBAO,13X,F6.3/
     5 50X,3HSRO,13X,F6.3/50X,4HLI2O,12X,F6.3//50X,3HSUM,12X,F7.3/1HO/1HO
     6 )
      PRINT 1122,Q,C,Z,OR,AB,AN,ALC
1122  FORMAT(1H1,56X,9HCIPW NORM/54X,16H(WEIGHT PERCENT)/1HO/55X,
     1 11HSALIC GROUP/
     2 44X,6HQUARTZ,21X,F6.3/
     3 44X,8HCORUNDUM,19X,F6.3/
     4 44X,6HZIRCON,21X,F6.3/
     5 44X,10HORTHOCLASE,17X,F6.3/
     6 44X,6HALBITE,21X,F6.3/
     7 44X,9HANORTHITE,18X,F6.3/
     8 44X,7HLEUCITE,20X,F6.3)
      PRINT 1123,ANE,AKP,HL,TH,ANC,SALG
1123  FORMAT(    44X,9HNEPHELINE,18X,F6.3/
     1 44X,12HKALIOPHILITE,15X,F6.3/
     2 44X,6HHALITE,21X,F6.3/
     3 44X,10HTHENARDITE,17X,F6.3/
     4 44X,16HSODIUM CARBONATE,11X,F6.3//56X,3HSUM,2X,F7.3/1HO/1HO)
      PRINT 1124,AC,ANS,AKS,DI,WO,HY,OL,CS,AMT
1124  FORMAT(1H ,55X,11HFEMIC GROUP/1HO/
     1 44X,6HACMITE,21X,F6.3/
     2 44X,19HSODIUM METASILICATE,8X,F6.3/
     3 44X,22HPOTASSIUM METASILICATE,5X,F6.3/
     4 44X,8HDICPSIDE,19X,F6.3/
     5 44X,12HWOLLASTONITE,15X,F6.3/
     6 44X,11HHYPERSTHENE,16X,F6.3/
     7 44X,7HOLIVINE,20X,F6.3/
     8 44X,21HCALCIUM ORTHOSILICATE,6X,F6.3/
     9 44X,9HMAGNETITE,18X,F6.3)
      PRINT 1125,HM,AIL,SP,PF,RU,AP,FR,PR,CC,CM,FEMG
1125  FORMAT(    44X,8HHEMATITE,19X,F6.3/
     1 44X,8HILMENITE,19X,F6.3/
     2 44X,6HSPHENE,21X,F6.3/
     3 44X,10HPEROVSKITE,17X,F6.3/
     4 44X,6HRUTILE,21X,F6.3/
     5 44X,7HAPATITE,20X,F6.3/
     6 44X,8HFLUORITE,19X,F6.3/
```

```
     7 44X,6HPYRITE,21X,F6.3/
     8 44X,7HCALCITE,20X,F6.3/
     9 44X,8HCHROMITE,19X,F6.3//56X,3HSUM,2X,F7.3)
       IF (1.+F1)1129,1127,1126
1126   PRINT 1131,R
1131   FORMAT(1H /1H /10X,52HRATIO MGO/FEO IN HYPERSTHENE DIOPSIDE AND OL
     1 IVINE = ,1PE12.4)
       GO TO 3333
1127   PRINT 1128
1128   FORMAT(1H /1H /10X,43HNO IRON IN HYPERSTHENE DIOPSIDE AND OLIVINE)
       GO TO 3333
1129   PRINT 1130
1130   FORMAT(1H /1H /10X,48HNO MAGNESIUM IN HYPERSTHENE DIOPSIDE AND OLI
     1 VINE)
3333   RETURN
       END

     M ULTIFILE END
```

Figure 3

Chemical Analysis 41

SiO_2	55.140	CO_2	0.000
Al_2O_3	0.660	SO_3	0.000
Fe_2O_3	3.480	Cl_2	0.000
FeO	4.730	F_2	0.000
MgO	26.660	S	0.000
CaO	8.390	Cr_2O_3	0.250
Na_2O	0.300	NiO	0.110
K_2O	0.000	CoO	0.000
TiO_2	0.000	BaO	0.000
P_2O_5	0.230	SrO	0.000
MnO	0.030	Li_2O	0.000
ZrO	0.000		
		Sum	99.980

CIPW Norm
(Weight Percent)

Salic Group		Femic Group	
Quartz	1.669	Acmite	0.000
Corundum	0.000	Sodium Metasilicate	0.000
Zircon	0.000	Potassium Metasilicate	0.000
Orthoclase	0.000	Diopside	32.670
Albite	2.535	Wollastonite	0.000
Anorthite	0.000	Hypersthene	57.409
Leucite	0.000	Olivine	0.000
Nepheline	0.000	Calcium Orthosilicate	0.000
Kaliophilite	0.000	Magnetite	5.046
Halite	0.000	Hematite	0.000
Thenardite	0.000	Ilmenite	0.000
Sodium Carbonate	0.000	Sphene	0.000
Sum	4.204	Perovskite	0.000
		Rutile	0.000
		Apatite	0.000
		Fluorite	0.000
		Pyrite	0.000
		Calcite	0.000
		Chromite	0.000
		Sum	95.125

Ratio MgO/FeO in hypersthene diopside and olivine = 1.4542E 01