

UNITED STATES DEPARTMENT OF THE INTERIOR
GEOLOGICAL SURVEY

CHEMANAL: A MULTICS Fortran program to
calculate chemical weathering data

by

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This report is preliminary and has not been
edited or reviewed for conformity
with U.S. Geological Survey standards

INTRODUCTION

This program is written in MULTICS Fortran, and calculates various chemical-weathering data from weight-percentage data. The input data file is a matrix with each row representing one sample, and each column representing one category of data. The input data matrix is composed of weight-percentage data for each sample (row) in the following format:

Column	Data	Format
1	Sample name	A8
2	Sample interval	A8*
3	bulk density	F6.2
4	SiO ₂	"
5	Al ₂ O ₃	"
6	Fe ₂ O ₃	"
7	FeO	"
8	MgO	"
9	CaO	"
10	Na ₂ O	"
11	K ₂ O	"
12	TiO ₂	"
13	P ₂ O ₅	"
14	MnO	"
15	CO ₂	"
16	H ₂ O ⁺	"
17	H ₂ O ⁻	"
18	Sum (of wt %'s)	"

*If (and only if) the first four spaces in this field are blank, the program treats the sample as a sample of the unweathered parent material, and calculates data normalized for the composition of the parent material. (See (2) and (5) below.)

To run the program, type "chemanal" (without quotes). The program will prompt the user for the name of the input data file, the starting and ending row numbers, the type of output, and the output file names.

Depending on user response to prompt questions, output files with the following types of data will be produced:

1. Weight percentages: This is the input data and will always be included in the output. TiR (ratio of TiO₂ in the unweathered parent material to that in the weathered sample) is calculated and included.
2. Molecular percentages, molecular ratios, and molecular ratios normalized to the composition of the parent material. Molecular ratios include:
 - (1) wPI and PI--weathering potential index and product index (Reiche, 1943,1950).
 - (2) Parkin--Parkinson's (1970) index.
 - (3) Si:R₂ and ba:R₂--Ratios of SiO₂ and bases (sum of Na₂O, K₂O, CaO, and MgO), respectively, to R₂O₃ (sum of Al₂O₃, Fe₂O₃, and TiO₂) (Jenny, 1941).
 - (4) Fe₃Fe₂--Ratio of Fe₂O₃ to FeO.
 - (5) TriSi, TriR₂, and TriBas--Percentages of SiO₂, R₂O₃, and bases, respectively, for a triangular diagram with their sum as 100 percent.
3. Standard-cell cations -- cations in a standard cell containing 160 oxygens (Barth, 1948).
4. weights, assuming isovolumetric weathering, calculated from bulk densities.
5. weights, assuming TiO₂ constant, calculated from the ratio of TiO₂ in the unweathered parent material to that in the weathered sample. Weights, assuming TiO₂ constant, normalized to the composition of the parent material, are also calculated.

Notes:

1. The program makes no provision for qualified data (for example, "less than").
2. The program treats FeO and Fe₂O₃ separately. If these two are to be combined, the combination should be made by recalculating the original analysis before data entry.
3. Molecular percentages and standard-cell cations are calculated using only H₂O⁺, not H₂O⁻.
4. The calculations for normalized molecular ratios and weights assuming TiO₂ constant require that a parent-material reference sample be identified (input data matrix, column 2).

REFERENCES

- Barth, T.W., 1948, Oxygen in rocks: A basis for petrographic calculations: *Journal of Geology*, v. 56, p. 50-61.
- Jenny, Hans, 1941, *Factors of soil formation*: New York, McGraw Hill, 281 p.
- Parker, A., 1970, An index of weathering for silicate rocks: *Geology Magazine*, v. 107, p. 501-504.
- Reiche, Parry, 1943, Graphical representation of chemical weathering: *Journal of Sedimentary Petrology*, v. 13, p. 58-68.
- _____, 1950, A survey of weathering processes and products: *New Mexico University Publications in Geology*, no. 3, 95p.

SAMPLE PROGRAM RUN

```
chemanal
Input data file?
? data1
Starting row number?
? 1
Ending row number?
? 14
Row 1 to row 14; number of rows= 14
Output file name for weight percentage data?
? wpc1
Do you want molecular percentages and ratios? (0=no,1=yes)
? 1
Output file name for molecular percentages?
? mp1
Output file name for molecular ratios?
? mr1
Output file name for normalized molecular ratios?
? nmr1
Do you want standard cell cations? (0=no,1=yes)
? 1
Output file name for standard cell cations?
? ssc1
Do you want weights per unit volume? (0=no,1=yes)
? 1
Output file name for weights per unit volume?
? wuv1
Do you want weights assuming TiO2 constant? (0=no,1=yes)
? 1
Output file name for weights assuming TiO2 constant?
? wtc1
Output file name for normalized weights assuming TiO2 constant?
? nwtc1
    Output file names:
wpc1
mp1
mr1
nmr1
ssc1
wuv1
wtc1
nwtc1
Do you want to run the program again for another set of rows (sam-
ples)? (0=no, 1=yes)
? 1
Input data file?
? data1
Starting row number?
? 15
Ending row number?
? 21
```

Row 15 to row 21; number of rows= 7
Output file name for weight percentage data?
? wpc2
Do you want molecular percentages and ratios? (0=no,1=yes)
? 0
Do you want standard cell cations? (0=no,1=yes)
? 1
Output file name for standard cell cations?
? ssc2
Do you want weights per unit volume? (0=no,1=yes)
? 1
Output file name for weights per unit volume?
? wuv2
Do you want weights assuming TiO2 constant? (0=no,1=yes)
? 0
 Output file names:
wpc2
ssc2
wuv2
Do you want to run the program again for another set of rows (samples)? (0=no, 1=yes)
? 0

STUP

Note: Input and output file names are arbitrary, supplied by the user. Examples of the input and output for this sample program run are given in appendixes 1 and 2, respectively.

PROGRAM LISTING

```

c *****
c *
c *      DATA ENTRY SECTION      *
c *
c *****
c
c Logical devices: 0=terminal, 1=working directory
c
      common wpc(100,25),tmpc(100,25),xmpc(100,25),tsso(100,25)
      common tssi(100,25),ssc(100,25),wuv(100,25),wtic(100,25)
      common norm(50),xnmpr(100,15),xntic(100,25),xmpr(100,15)
      common outnam(10),twpc(100,25)
      double precision wpc wtic
      character namseg*10
      character outnam*10
      open(0,prompt=.true.)
c
c *****
c Entry of weight percentages
c *****
c
700  write (0,10)
10   format ("Input data file?")
      read (0,11) namseg
11   format (a10)
      write (0,14)
14   format ("Starting row number?")
      read (0,15) nr1
15   format (v)
      write (0,16)
16   format ("Ending row number?")
      read (0,17) nr2
17   format (v)
      n=(nr2-nr1)+1
      write(0,24) nr1,nr2,n
24   format("Row ",I3," to row ",I3,"; number of rows=",I3)
      open(1,file=namseg,form="formatted",mode="in")
      read (1,19) ((twpc(k,j),j=1,20),k=1,nr2)
19   format (4a4,16f6.2)
      do 600 k=1,n
      do 601 j=1,20
      wpc(k,j)=twpc(k-1+nr1,j)
601  continue
600  continue
      close(1)
c
c *****
c Identification of unweathered parent material samples
c *****
c

```



```

      m=1
      data blanks/"      "/
      do 800 k=1,n
      if(wpc(k,3).ne.blanks) go to 800
      norm(m)=k
      m=m+1
800  continue
c
c *****
c Calculation of TiR
c *****
c
      m=1
      do 900 k=1,n
      mm=norm(m)
      wpc(k,21)=wpc(mm,14)/wpc(k,14)
      if (k-mm) 900,901,900
901  m=m+1
900  continue
c
c *****
c Weight percentages output
c *****
c
      nn=1
      write (0,66)
66  format("Output file name for weight percentage data?")
      read (0,11) namseg
      outnam(nn)=namseg
      open(1,file=namseg,form="formatted",mode="out")
      write (1,65)
65  format("WEIGHT PERCENT DATA")
      write (1,20)
20  format (2x,"Sample Interv.  BD  SiO2 Al2O3 Fe2O3  FeO
cMgO  CaO  Na2O  K2O  TiO2  P2O5  MnO  CO2  H2O+  H2O-
c Sum  TiR")
      write (1,21) ((wpc(k,j),j=1,21),k=1,n)
21  format (4a4,15f6.2,1x,2f6.2)
      close(1)
c
c *****
c *          CALCULATIONS SECTION          *
c *          *          *
c *****
c
c *****
c Molecular weight conversions
c *****
c
      do 101 k=1,n
c SiO2
      tmpc(k,1) = wpc(k,6)/60.

```

```

c Al2O3
  tmpc(k,2) = wpc(k,7)/102.
c Fe2O3
  tmpc(k,3) = wpc(k,8)/159.6
c FeO
  tmpc(k,4) = wpc(k,9)/71.8
c MgO
  tmpc(k,5) = wpc(k,10)/40.3
c CaO
  tmpc(k,6) = wpc(k,11)/56.
c Na2O
  tmpc(k,7) = wpc(k,12)/62.
c K2O
  tmpc(k,8) = wpc(k,13)/94.2
c TiO2
  tmpc(k,9) = wpc(k,14)/79.2
c P2O5
  tmpc(k,10) = wpc(k,15)/142.
c MnO
  tmpc(k,11) = wpc(k,16)/70.9
c CO2
  tmpc(k,12) = wpc(k,17)/44.
c H2O+
  tmpc(k,13) = wpc(k,18)/18.
c Hydrous totals (H2O+ only)
  tot = 0.0
  do 201 j=1,13
    tot = tot + tmpc(k,j)
201  continue
  tmpc(k,14) = tot
c Anhydrous totals
  tot = 0.0
  do 202 j=1,12
    tot = tot + tmpc(k,j)
202  continue
  tmpc(k,15) = tot
101  continue
c
c *****
c Molecular percentages and ratios
c *****
c
  write (0,31)
31  format("Do you want molecular percentages and ratios? (0=no
      c,1=yes)")
  read(0,32) itest1
32  format (v)
  if (itest1) 302,302,301
c
c ***** Molecular percentages *****
c
301  continue
  do 111 k=1,n

```

```

        tot=0.0
        xmpc(k,1) = wpc(k,1)
        xmpc(k,2) = wpc(k,2)
        do 203 j=3,15
        xmpc(k,j) = 100.*(tmpc(k,j-2)/tmpc(k,14))
        tot=tot+xmpc(k,j)
203    continue
        xmpc(k,10)=tot
c
c ***** Molecular ratios *****
c
        xmpr(k,1) = wpc(k,1)
        xmpr(k,2) = wpc(k,2)
c sigma bases
        xmpr(k,3) = xmpc(k,7)+xmpc(k,8)+xmpc(k,9)+xmpc(k,10)
c sigma R2U3
        xmpr(k,4) = xmpc(k,4)+xmpc(k,5)+0.5*xmpc(k,6)+xmpc(k,11)
c WPI
        xmpr(k,5) = 100.*((xmpr(k,3)-xmpc(k,15))/(xmpr(k,3)+xmpr(k,
c4)+xmpc(k,3)))
c PI
        xmpr(k,6) = 100.*((xmpc(k,3))/(xmpc(k,3)+xmpr(k,4)))
c Parker's Index
        xmpr(k,7) = 1.*((xmpc(k,7)/0.9)+(xmpc(k,8)/0.7+(xmpc(k,9)/
c0.35)+(xmpc(k,10)/0.25))
c SiU2/R2O3
        xmpr(k,8) = xmpc(k,3)/xmpr(k,4)
c bases/R2U3
        xmpr(k,9) = xmpr(k,3)/xmpr(k,4)
c Fe2O3:FeU
        if (xmpc(k,5)) 809,810,809
809    if (xmpc(k,6)) 814,810,814
810    xmpr(k,10)=0.0
        go to 811
814    xmpr(k,10)=xmpc(k,5)/xmpc(k,6)
c SiU2-R2O3-bases triangular diagram percents
811    tot=xmpc(k,3)+xmpr(k,3)+xmpr(k,4)
        xmpr(k,11)=100.*xmpc(k,3)/tot
        xmpr(k,12)=100.*xmpr(k,4)/tot
        xmpr(k,13)=100.*xmpr(k,3)/tot
111    continue
c
c ***** normalized molecular ratios *****
c
        m=1
        do 801 k=1,n
        xnmpr(k,1)=wpc(k,1)
        xnmpr(k,2)=wpc(k,2)
        mm=norm(m)
        do 803 j=3,13
        if (xnmpr(mm,j)) 812,813,812
813    xnmpr(k,j)=0.0
        go to 803

```

```

812  xmpr(k,j)=xmpr(k,j)/xmpr(mm,j)
803  continue
      if (k=mm) 801,802,802
802  m=m+1
801  continue
c
c ***** Output *****
c
      nn=nn+1
      write(0,70)
70   format("Output file name for molecular percentages?")
      read(0,11) namseg
      outnam(nn)=namseg
      open(1,file=namseg,form="formatted",mode="out")
      write(1,60)
60   format("MOLECULAR PERCENTAGES")
      write(1,22)
22   format(2x,"Sample  SiO2  Al2O3  Fe2O3   FeO   MgO   CaO   Na2O
c    K2O  TiO2  P2O5   MnO   CO2  H2O+  Sum")
      write (1,23) ((xmpc(k,j)),j=1,16),k=1,n)
23   format (2a4,13f6.2,1x,f6.2)
      close (1)
      nn=nn+1
      write(0,71)
71   format("Output file name for molecular ratios?")
      read(0,11) namseg
      outnam(nn)=namseg
      open(1,file=namseg,form="formatted",mode="out")
      write(1,61)
61   format("MOLECULAR RATIOS")
      write (1,12)
12   format (2x,"Sample  Bases   R2O3   WPI       PI  Parkin  Si:R
c2  Ba:K2 Fe3Fe2  TriSi  IriR2  IriBas")
      write (1,13) ((xmpr(k,j)),j=1,13),k=1,n)
13   format (2a4,11f7.2)
      close(1)
      nn=nn+1
      write(0,72)
72   format("Output file name for normalized molecular ratios?")
      read (0,11) namseg
      outnam(nn) =namseg
      open(1,file=namseg,form="formatted",mode="out")
      write(1,80)
80   format("NORMALIZED MOLECULAR RATIOS")
      write(1,12)
      write(1,13) ((xnmpr(k,j)),j=1,13),k=1,n)
      close(1)
c
c *****
c Standard cell cations
c *****
c
302  write(0,33)

```

```

33   format("Do you want standard cell cations? (0=no,1=yes)")
      read(0,34) itest2
34   format(v)
      if (itest2) 304,304,303
c
c ***** Calculations *****
c
303   do 102 k=1,n
c Si
      tssso(k,1) = tmpc(k,1)*2.0/tmpc(k,14)
      tsssi(k,1) = tmpc(k,1)/tmpc(k,14)
c Al
      tssso(k,2) = (tmpc(k,2)*3)/tmpc(k,14)
      tsssi(k,2) = (tmpc(k,2)*2)/tmpc(k,14)
c Fe3
      tssso(k,3) = (tmpc(k,3)*3)/tmpc(k,14)
      tsssi(k,3) = (tmpc(k,3)*2)/tmpc(k,14)
c Fe2
      tssso(k,4) = (tmpc(k,4))/tmpc(k,14)
      tsssi(k,4) = (tmpc(k,4))/tmpc(k,14)
c Mg
      tssso(k,5) = tmpc(k,5)/tmpc(k,14)
      tsssi(k,5) = tmpc(k,5)/tmpc(k,14)
c Ca
      tssso(k,6) = tmpc(k,6)/tmpc(k,14)
      tsssi(k,6) = tmpc(k,6)/tmpc(k,14)
c Na
      tssso(k,7) = tmpc(k,7)/tmpc(k,14)
      tsssi(k,7) = tmpc(k,7)*2.0/tmpc(k,14)
c K
      tssso(k,8) = tmpc(k,8)/tmpc(k,14)
      tsssi(k,8) = tmpc(k,8)*2.0/tmpc(k,14)
c Ti
      tssso(k,9) = tmpc(k,9)*2.0/tmpc(k,14)
      tsssi(k,9) = tmpc(k,9)/tmpc(k,14)
c P
      tssso(k,10) = (tmpc(k,10)*5)/tmpc(k,14)
      tsssi(k,10) = (tmpc(k,10)*2)/tmpc(k,14)
c Mn
      tssso(k,11) = tmpc(k,11)/tmpc(k,14)
      tsssi(k,11) = tmpc(k,11)/tmpc(k,14)
c C
      tssso(k,12) = tmpc(k,12)*2.0/tmpc(k,14)
      tsssi(k,12) = tmpc(k,12)/tmpc(k,14)
c H
      tssso(k,13) = tmpc(k,13)/tmpc(k,14)
      tsssi(k,13) = tmpc(k,13)*2.0/tmpc(k,14)
c Sum of 0
      tot=0.0
      do 204 j=1,13
      tot = tot + tssso(k,j)
204   continue
      tssso(k,14) =tot

```

```

c Cations
  ssc(k,1) = wpc(k,1)
  ssc(k,2) = wpc(k,2)
  do 205 j=3,15
  ssc(k,j) = tssi(k,j-2)*160.0/tsso(k,14)
205  continue
  tot = 0.0
  do 206 j=3,15
  tot = tot + ssc(k,j)
206  continue
  ssc(k,16) = tot
102  continue
c
c ***** Output *****
c
  nn=nn+1
  write(0,73)
73  format("Output file name for standard cell cations?")
  read(0,11) namseg
  outnam(nn)=namseg
  open(1,file=namseg,form="formatted",mode="out")
  write(1,62)
62  format("STANDARD CELL CATIONS")
  write (1,28)
28  format(2x,"Sample  Si    Al    Fe3+  Fe2+  Mg    Ca    Na
c      K    Tj    P      Mn    C      H      Sum")
  write (1,29) ((ssc(k,j),j=1,16),k=1,n)
29  format (2a4,13f6.2,1x,f6.2)
  close(1)
c
c *****
c weights per unit volume
c *****
c
304  write(0,35)
35  format("Do you want weights per unit volume? (0=no,1=yes)")
  read(0,36) itest3
36  format(v)
  if (itest3) 306,306,305
c
c ***** Calculations *****
c
305  do 103 k=1,n
  wuv(k,1) = wpc(k,1)
  wuv(k,2) = wpc(k,2)
  wuv(k,3) = wpc(k,5)
  do 207 j=4,17
  wuv(k,j)=wpc(k,j+2)*wpc(k,5)
207  continue
  tot = 0.0
  do 208 j=4,17
  tot =tot + wuv(k,j)
208  continue

```

```

        wuv(k,18) = tot
103  continue
c
c ***** Output *****
c
        nn=nn+1
        write(0,74)
74  format("Output file name for weights per unit volume?")
        read(0,11) namseg
        outnam(nn)=namseg
        open(1,file=namseg,form="formatted",mode="out")
        write(1,63)
63  format("WEIGHTS PER UNIT VOLUME")
        write(1,57)
57  format(2x,"Sample  BD   SiO2  Al2O3 Fe2O3   FeO   MgO   Ca
cU  Na2O  K2O  TiO2  P2O5   MnO   CO2  H2O+  H2O-  Sum")
        write(1,58) ((wuv(k,j),j=1,18),k=1,n)
58  format(2a4,f6.2,1x,14f6.2,1x,f6.2)
        close(1)
c
c *****
c Weights assuming TiO2 constant
c *****
c
306  write (0,41)
41  format("Do you want weights assuming TiO2 constant? (0=no,1
c=yes)")
        read(0,42) itest4
42  format(v)
        if (itest4) 308,308,307
c
c ***** Calculations *****
c
307  do 104 k=1,n
        wtic(k,1)=wpc(k,1)
        wtic(k,2)=wpc(k,2)
        wtic(k,3)=wpc(k,21)
        do 209 j=4,18
            wtic(k,j)=wpc(k,j+2)*wpc(k,21)
209  continue
104  continue
c
c ***** Normalized weights, TiO2 constant *****
c
        m=1
        do 804 k=1,n
            xntic(k,1)=wpc(k,1)
            xntic(k,2)=wpc(k,2)
            xntic(k,3)=wpc(k,21)
            mm=norm(m)
            do 805 j=4,18
                if (wtic(k,j)) 808,807,808
807  wtic(k,j)=0.0

```

```

      go to 805
808  xntic(k,j)=wtic(k,j)/wtic(mm,j)
805  continue
      if (k=mm) 804,806,806
806  m=m+1
804  continue
c
c ***** Output *****
c
      nn=nn+1
      write(0,75)
75  format("Output file name for weights assuming TiO2 constant
c?")
      read(0,11) namseg
      outnam(nn)=namseg
      open(1,file=namseg,form="formatted",mode="out")
      write(1,64)
84  format("WEIGHTS ASSUMING TiO2 CONSTANT")
      write(1,43)
43  format(2x,"Sample  TiR   SiO2 Al2O3 Fe2O3   FeO   MgO   CaO
c Na2O  K2O  TiO2  P2O5   MnO   CO2  H2O+  H2O-   Sum")
      write(1,44) ((wtic(k,j),j=1,18),k=1,n)
44  format(2a4,14f6.2,1x,f6.2,1x,f6.2)
      close(1)
      nn=nn+1
      write(0,76)
76  format("Output file name for normalized weights assuming Ti
cO2 constant?")
      read(0,11) namseg
      outnam(nn)=namseg
      open(1,file=namseg,form="formatted",mode="out")
      write(1,82)
82  format("NORMALIZED WEIGHTS ASSUMING TiO2 CONSTANT")
      write(1,43)
      write(1,44) ((xntic(k,j),j=1,18),k=1,n)
      close(1)
c
c
c *****
c *
c *          CLOSING STATEMENTS          *
c *
c *****
c
308  write (0,77)
77  format("      Output file names:")
      write (0,11) (outnam(kk),kk=1,nn)
      write(0,45)
45  format("Do you want to run the program again for another se
ct of rows (samples)? (0=no, 1=yes)")
      read(0,15) itest5
      if (itest5) 701,701,700
701  stop
      end

```


APPENDIX 1---Input Data For Sample Program Run

109-a1	0.0-0.5	2.1	35.6	17.6	16.0	4.4	2.8	3.2	0.3	0.5	4.8	0.4	0.2	0.1	9.5	3.4	98.8
109-a2	0.5-1.4	2.4	38.	12.	21.	0.	5.3	7.2	1.01	0.81	3.9	0.	0.18	0.	10.7	0.	100.
109-a3	1.4-2.0	2.6	41.	12.	18.	0.	5.3	8.3	1.84	0.81	3.1	0.	0.20	0.	9.5	0.	100.
109-a4	>2.0	2.8	53.7	14.1	1.9	9.8	4.2	8.1	2.8	1.5	2.2	0.4	0.2	0.1	1.2	0.3	100.5
105-a1	0.0-0.5	2.7	53.6	16.8	7.0	3.0	2.7	5.4	2.2	1.1	2.0	0.3	0.2	0.1	4.1	1.8	100.3
105-a2	>0.5	2.8	53.4	15.0	2.0	9.0	4.2	8.1	2.8	1.3	2.1	0.4	0.2	0.1	1.2	0.5	100.3
104-a1	0.0-0.5	2.3	43.8	11.5	4.4	14.8	8.5	6.4	2.1	0.7	3.4	0.3	0.2	0.1	2.5	0.3	99.5
104-a2	0.5-1.0	2.6	43.9	11.9	3.2	15.3	8.7	7.9	2.4	0.5	3.1	0.4	0.2	0.1	1.1	0.1	98.8
104-a3	>1.0	2.8	46.5	15.8	2.0	2.1	6.9	9.1	3.0	0.5	2.4	0.3	0.2	0.1	1.1	0.2	99.6
102-a1	0.0-0.7	2.4	36.	9.6	23.	0.	6.4	6.6	0.96	0.74	3.8	0.	0.26	0.	12.6	0.	100.
102-a2	0.7-1.5	2.5	40.	11.	20.	0.	6.05	7.7	1.76	0.74	3.2	0.	0.24	0.	9.3	0.	100.
102-a3	>1.5	2.8	48.	14.	14.	0.	4.18	8.5	3.05	0.96	2.2	0.	0.19	0.	5.0	0.	100.
98-a1	0.0-0.4	2.5	46.1	13.2	5.5	10.5	6.5	7.9	2.3	0.7	3.3	0.3	0.2	0.1	1.9	0.1	98.6
98-a2	>0.4	2.8	48.8	15.9	4.0	9.9	6.5	9.2	2.9	0.5	2.4	0.3	0.2	0.1	0.4	0.1	101.2
118-a1	0.0-2.0	1.7	39.	16.	19.	0.	1.60	0.29	0.31	0.72	2.6	0.	0.09	0.	20.4	0.	100.
118-a2	2.6-5.2	2.0	39.	7.2	27.	0.	2.45	0.49	0.49	0.95	3.4	0.	0.09	0.	18.9	0.	100.
118-a3	5.2-7.8	2.4	47.	7.5	21.	0.	4.98	1.5	0.95	1.5	3.0	0.	0.12	0.	12.4	0.	100.
118-a4	>7.8	2.7	57.	15.	6.6	0.	3.90	7.5	3.6	1.2	1.1	0.	0.11	0.	4.0	0.	100.
95-a1	0.0-0.3	2.4	47.6	16.8	6.0	3.2	6.6	4.7	1.8	1.9	1.1	0.17	0.23	0.01	6.6	2.4	99.
95-a2	0.3-0.7	2.5	52.8	11.6	4.3	6.4	10.9	6.3	2.0	1.6	1.3	0.11	0.19	0.01	2.2	1.1	101.
95-a3	>0.7	2.8	54.5	16.3	2.6	4.6	8.7	8.4	3.2	1.2	0.82	0.25	0.13	0.02	0.42	0.30	101.

APPENDIX 2--Output Data From Sample Program Run
(See Introduction for explanation.)

File name: wpc1

WEIGHT PERCENT DATA

Sample	Interv.	BD	SiO2	Al2O3	Fe2O3	FeO	MgO	CaO	Na2O	K2O	TiO2	P2O5	MnO	CO2	H2O+	H2O-	Sum	TiR
109-a1	0.0-0.5	2.10	35.60	17.60	16.00	4.40	2.80	3.20	0.30	0.50	4.80	0.40	0.20	0.10	9.50	3.40	98.80	0.46
109-a2	0.5-1.4	2.40	38.00	12.00	21.00	0.00	5.30	7.20	1.01	0.81	3.90	0.00	0.18	0.00	10.70	0.00	100.00	0.56
109-a3	1.4-2.0	2.60	41.00	12.00	18.00	0.00	5.30	8.30	1.84	0.81	3.10	0.00	0.20	0.00	9.50	0.00	100.00	0.71
109-a4	>2.0	2.80	53.70	14.10	1.90	9.80	4.20	8.10	2.80	1.50	2.20	0.40	0.20	0.10	1.20	0.30	100.50	1.00
105-a1	0.0-0.5	2.70	53.60	16.80	7.00	3.00	2.70	5.40	2.20	1.10	2.00	0.30	0.20	0.10	4.10	1.80	100.30	1.05
105-a2	>0.5	2.80	53.40	15.00	2.00	9.00	4.20	8.10	2.80	1.30	2.10	0.40	0.20	0.10	1.20	0.50	100.30	1.00
104-a1	0.0-0.5	2.30	43.80	11.50	4.40	14.80	8.50	6.40	2.10	0.70	3.40	0.30	0.20	0.10	2.50	0.30	99.50	0.71
104-a2	0.5-1.0	2.60	43.90	11.90	3.20	15.30	8.70	7.90	2.40	0.50	3.10	0.40	0.20	0.10	1.10	0.10	98.80	0.77
104-a3	>1.0	2.80	46.50	15.80	2.00	2.10	6.90	9.10	3.00	0.50	2.40	0.00	0.26	0.10	0.50	0.20	99.60	1.00
102-a1	0.0-0.7	2.40	36.00	9.60	23.00	0.00	6.40	6.60	0.96	0.74	3.80	0.00	0.26	0.00	12.60	0.00	100.00	0.58
102-a2	0.7-1.5	2.50	40.00	11.00	20.00	0.00	6.05	7.70	1.76	0.74	3.20	0.00	0.24	0.00	9.30	0.00	100.00	0.69
102-a3	>1.5	2.80	48.00	14.00	14.00	0.00	4.18	8.50	3.05	0.96	2.20	0.00	0.19	0.00	5.00	0.00	100.00	1.00
98-a1	0.0-0.4	2.50	46.10	13.20	5.50	10.50	6.50	7.90	2.30	0.70	3.30	0.30	0.20	0.10	1.90	0.10	98.60	0.73
98-a2	>0.4	2.80	48.80	15.90	4.00	9.90	6.50	9.20	2.90	0.50	2.40	0.30	0.20	0.10	0.40	0.10	101.20	1.00

File name: wpc2

WEIGHT PERCENT DATA

Sample	Interv.	BD	SiO2	Al2O3	Fe2O3	FeO	MgO	CaO	Na2O	K2O	TiO2	P2O5	MnO	CO2	H2O+	H2O-	Sum	TiR
118-a1	0.0-2.6	1.70	39.00	16.00	19.00	0.00	1.60	0.29	0.31	0.72	2.60	0.00	0.09	0.00	20.40	0.00	100.00	0.42
118-a2	2.6-5.2	2.00	39.00	7.20	27.00	0.00	2.45	0.49	0.49	0.95	3.40	0.00	0.09	0.00	18.90	0.00	100.00	0.32
118-a3	5.2-7.8	2.40	47.00	7.50	21.00	0.00	4.98	1.50	0.95	1.50	3.00	0.00	0.12	0.00	12.40	0.00	100.00	0.37
118-a4	>7.8	2.70	57.00	15.00	6.60	0.00	3.90	7.50	3.60	1.20	1.10	0.00	0.11	0.00	4.00	0.00	100.00	1.00
95-a1	0.0-0.3	2.40	47.60	16.80	6.00	3.20	6.60	4.70	1.80	1.90	1.10	0.17	0.23	0.01	6.60	2.40	99.00	0.75
95-a2	0.3-0.7	2.50	52.80	11.60	4.30	6.40	10.90	6.30	2.00	1.60	1.30	0.11	0.19	0.01	2.20	1.10	101.00	0.63
95-a3	>0.7	2.80	54.50	16.30	2.60	4.60	8.70	8.40	3.20	1.20	0.82	0.25	0.13	0.02	0.42	0.30	101.00	1.00

File name: mp1

MOLECULAR PERCENTAGES

Sample	SiO2	Al2O3	Fe2O3	FeO	MgO	CaO	Na2O	K2O	TiO2	P2O5	MnO	CO2	H2O+	Sum
109-a1	35.73	10.39	6.04	3.69	4.18	3.44	0.29	0.32	3.65	0.17	0.17	0.14	31.78	100.00
109-a2	34.92	6.49	7.25	0.00	7.25	7.09	0.90	0.47	2.71	0.00	0.14	0.00	32.77	100.00
109-a3	37.93	6.53	6.26	0.00	7.30	8.23	1.65	0.48	2.17	0.00	0.16	0.00	29.30	100.00
109-a4	56.15	8.67	0.75	8.56	6.54	9.07	2.83	1.00	1.74	0.18	0.18	0.14	4.18	100.00
105-a1	55.33	10.20	2.72	2.59	4.15	5.97	2.20	0.72	1.56	0.13	0.17	0.14	14.11	100.00
105-a2	56.19	9.28	0.79	7.91	6.58	9.13	2.85	0.87	1.67	0.18	0.18	0.14	4.21	100.00
104-a1	44.73	6.91	1.69	12.63	12.92	7.00	2.08	0.46	2.63	0.13	0.17	0.14	8.51	100.00
104-a2	46.00	7.33	1.26	13.40	13.57	8.87	2.43	0.33	2.46	0.18	0.18	0.14	3.84	100.00
104-a3	54.41	10.88	0.88	2.05	12.02	11.41	3.40	0.37	2.13	0.15	0.20	0.16	1.95	100.00
102-a1	31.75	4.98	7.63	0.00	8.40	6.24	0.82	0.42	2.54	0.00	0.19	0.00	37.04	100.00
102-a2	37.37	6.04	7.02	0.00	8.41	7.71	1.59	0.44	2.26	0.00	0.19	0.00	28.96	100.00
102-a3	48.54	8.33	5.32	0.00	6.29	9.21	2.98	0.62	1.69	0.00	0.16	0.00	16.85	100.00
98-a1	48.64	8.19	2.18	9.26	10.21	8.93	2.35	0.47	2.64	0.13	0.18	0.14	6.68	100.00
98-a2	51.82	9.93	1.60	8.78	10.28	10.47	2.98	0.34	1.93	0.13	0.18	0.14	1.42	100.00

File name: mr1

MOLECULAR RATIOS

Sample	Bases	K2O3	WPI	PI	Parkin	Si:R2	Ba:R2	Fe3Fe2	TriSi	TriR2	TriBas
109-a1	8.24	21.92	-35.74	61.97	11.68	1.63	0.38	1.64	54.23	33.27	12.50
109-a2	15.71	16.46	-25.43	67.97	22.65	2.12	0.95	0.00	52.05	24.53	23.42
109-a3	17.65	14.96	-16.51	71.71	26.48	2.53	1.18	0.00	53.77	21.21	25.02
109-a4	19.45	15.44	16.77	78.43	32.32	3.04	1.26	0.09	61.68	16.96	21.36
105-a1	13.04	15.78	-1.27	77.81	22.32	3.51	0.83	1.05	65.75	18.75	15.50
105-a2	19.44	15.71	16.67	78.15	31.99	3.58	1.24	0.10	61.52	17.20	21.28
104-a1	22.46	17.54	16.46	71.83	32.12	2.55	1.28	0.13	52.79	20.70	26.50
104-a2	25.21	17.75	24.02	72.15	36.04	2.59	1.42	0.09	51.71	19.96	28.34
104-a3	27.20	14.91	26.16	78.49	40.85	3.65	1.82	0.43	56.37	15.45	28.18
102-a1	15.87	15.14	-33.72	67.70	22.25	2.10	1.05	0.00	50.58	24.13	25.29
102-a2	18.15	15.33	-15.25	70.90	26.67	2.44	1.18	0.00	52.74	21.64	25.62
102-a3	19.11	15.34	2.71	75.99	31.15	3.17	1.25	0.00	58.49	18.48	23.02
98-a1	21.96	17.64	17.31	73.58	32.69	2.76	1.24	0.24	55.12	19.99	24.89
98-a2	24.06	17.85	24.16	74.38	36.24	2.90	1.35	0.18	55.28	19.05	25.67

File name: nmri

NORMALIZED MOLECULAR RATIOS

Sample	Bases	K2O3	WPI	PI	Parkin	Si:R2	Ba:R2	Fe3Fe2	TriSi	TriR2	TriBas
109-a1	0.42	1.42	-2.13	0.79	0.36	0.45	0.30	18.76	0.88	1.96	0.59
109-a2	0.81	1.07	-1.52	0.87	0.70	0.58	0.76	0.00	0.84	1.45	1.10
109-a3	0.91	0.97	-0.98	0.91	0.82	0.70	0.94	0.00	0.87	1.25	1.17
109-a4	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
105-a1	0.67	1.00	-0.08	1.00	0.70	0.98	0.67	10.50	1.07	1.09	0.73
105-a2	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
104-a1	0.83	1.18	0.63	0.92	0.79	0.70	0.70	0.31	0.94	1.34	0.94
104-a2	0.93	1.19	0.92	0.92	0.88	0.71	0.78	0.22	0.92	1.29	1.01
104-a3	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
102-a1	0.83	0.99	-12.43	0.89	0.71	0.66	0.84	0.00	0.86	1.51	1.10
102-a2	0.95	1.00	-5.62	0.93	0.86	0.77	0.95	0.00	0.90	1.17	1.11
102-a3	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	1.00	1.00
98-a1	0.91	0.99	0.72	0.99	0.90	0.95	0.92	1.30	1.00	1.05	0.97
98-a2	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

File name: ssc1

STANDARD CELL CATIONIS

Sample	Si	Al	Fe3+	Fe2+	Mg	Ca	Na	K	Ti	P	Mn	C	H	Sum
109-a1	35.04	19.22	11.16	3.41	3.87	3.18	0.54	0.59	3.37	0.31	0.16	0.13	58.77	157.75
109-a2	33.84	12.57	14.06	0.00	7.03	6.87	1.74	0.92	2.63	0.00	0.14	0.00	63.52	143.31
109-a3	36.03	12.61	12.09	0.00	7.05	7.94	3.18	0.92	2.10	0.00	0.15	0.00	56.58	139.26
109-a4	50.59	15.63	1.35	7.72	5.89	8.18	5.11	1.80	1.57	0.32	0.16	0.13	7.54	105.97
105-a1	48.27	17.80	4.74	2.26	3.02	5.21	3.83	1.26	1.36	0.23	0.15	0.12	24.62	113.48
105-a2	50.26	16.01	1.42	7.08	5.89	8.17	5.10	1.56	1.50	0.32	0.16	0.13	16.48	115.99
104-a1	45.32	13.38	5.27	12.23	12.52	6.78	4.02	0.88	2.55	0.25	0.17	0.13	16.48	115.99
104-a2	44.20	14.10	2.42	12.87	13.04	8.52	4.68	0.64	2.36	0.34	0.17	0.14	7.38	110.88
104-a3	48.15	19.25	1.56	1.82	10.64	10.10	6.01	0.66	1.88	0.26	0.18	0.14	3.45	104.09
102-a1	31.85	9.99	15.30	0.00	8.43	6.26	1.64	0.83	2.55	0.00	0.19	0.00	74.31	151.35
102-a2	36.07	11.07	13.56	0.00	8.12	7.44	3.07	0.85	2.19	0.00	0.18	0.00	55.90	139.05
102-a3	43.75	15.01	9.59	0.00	5.07	8.30	5.38	1.11	1.52	0.00	0.15	0.00	30.38	120.87
98-a1	45.06	15.18	4.04	8.58	9.46	8.27	4.35	0.87	2.44	0.25	0.17	0.13	12.38	111.18
98-a2	46.71	17.91	2.88	7.92	9.26	9.44	5.37	0.61	1.74	0.24	0.16	0.13	2.55	104.93

File name: ssc2

STANDARD CELL CATIONIS

Sample	Si	Al	Fe3+	Fe2+	Mg	Ca	Na	K	Ti	P	Mn	C	H	Sum
118-a1	30.72	14.83	11.25	0.00	1.88	0.24	0.47	0.72	1.55	0.00	0.06	0.00	107.12	168.85
118-a2	32.06	6.96	16.69	0.00	3.00	0.43	0.78	0.99	2.12	0.00	0.06	0.00	103.58	166.67
118-a3	40.04	7.52	13.45	0.00	6.32	1.37	1.57	1.63	1.94	0.00	0.09	0.00	70.43	144.35
118-a4	50.36	15.59	4.38	0.00	5.13	7.10	6.16	1.35	0.74	0.00	0.08	0.00	23.56	114.45
95-a1	43.19	17.93	4.09	2.43	8.92	4.57	3.16	2.20	0.76	0.13	0.18	0.01	39.92	127.48
95-a2	49.14	12.70	3.01	4.98	15.10	6.28	3.60	1.90	0.92	0.09	0.15	0.01	13.65	111.52
95-a3	50.20	17.66	1.80	3.54	11.93	8.29	5.71	1.41	0.57	0.19	0.10	0.03	2.58	104.02

File name: wuv1

WEIGHTS PER UNIT VOLUME

Sample	Rd	SiU2	Al2O3	Fe2O3	FeO	MgO	CaO	Na2O	K2O	TiO2	P2O5	MnO	CO2	H2O+	H2O-	Sum
109-a1	2.10	74.76	36.96	33.60	9.24	5.88	6.72	0.63	1.05	10.08	0.84	0.42	0.21	19.95	7.14	207.48
109-a2	2.40	91.20	28.80	50.40	0.00	12.72	17.28	2.42	1.94	9.36	0.00	0.43	0.00	25.68	0.00	240.24
109-a3	2.60	106.60	31.20	46.80	0.00	13.78	21.58	4.78	2.11	8.06	0.00	0.52	0.00	24.70	0.00	260.13
109-a4	2.80	150.36	39.48	5.32	27.44	11.76	22.68	7.84	4.20	6.16	1.12	0.56	0.28	3.36	0.84	281.40
105-a1	2.70	144.72	45.36	18.90	8.10	7.29	14.58	5.94	2.97	5.40	0.81	0.54	0.27	11.07	4.86	270.81
105-a2	2.80	149.52	42.00	5.60	25.20	11.76	22.68	7.84	3.64	5.88	1.12	0.56	0.28	3.36	1.40	280.84
104-a1	2.30	100.74	26.45	10.12	34.04	19.55	14.72	4.83	1.61	7.82	0.69	0.46	0.23	5.75	0.69	227.70
104-a2	2.60	114.14	30.94	8.32	39.78	22.62	20.54	6.24	1.30	8.06	1.04	0.52	0.26	2.86	0.26	256.88
104-a3	2.80	130.20	44.24	5.60	5.88	19.32	25.48	8.40	1.40	6.72	0.84	0.56	0.28	1.40	0.56	250.88
102-a1	2.40	86.40	23.04	55.20	0.00	15.36	15.84	2.30	1.78	9.12	0.00	0.62	0.00	30.24	0.00	239.90
102-a2	2.50	100.00	27.50	50.00	0.00	15.13	19.25	4.40	1.85	8.00	0.00	0.60	0.00	23.25	0.00	249.98
102-a3	2.60	134.40	39.20	39.20	0.00	11.70	23.80	8.54	2.69	6.16	0.00	0.53	0.00	14.00	0.00	280.22
98-a1	2.50	115.25	33.00	13.75	26.25	16.25	19.75	5.75	1.75	8.25	0.75	0.50	0.25	4.75	0.25	246.50
98-a2	2.80	136.64	44.52	11.20	27.72	18.20	25.76	8.12	1.40	6.72	0.84	0.56	0.28	1.12	0.28	283.36

File name: wuv2

WEIGHTS PER UNIT VOLUME

Sample	Rd	SiU2	Al2O3	Fe2O3	FeO	MgO	CaO	Na2O	K2O	TiO2	P2O5	MnO	CO2	H2O+	H2O-	Sum
118-a1	1.70	66.30	27.20	32.30	0.00	2.72	0.49	0.53	1.22	4.42	0.00	0.15	0.00	34.68	0.00	170.02
118-a2	2.00	78.00	14.40	54.00	0.00	4.90	0.98	0.98	1.90	6.80	0.00	0.18	0.00	37.80	0.00	199.94
118-a3	2.40	112.80	18.00	50.40	0.00	11.95	3.60	2.28	3.60	7.20	0.00	0.29	0.00	29.76	0.00	239.88
118-a4	2.70	153.90	40.50	17.82	0.00	10.53	20.25	9.72	3.24	2.97	0.00	0.30	0.00	10.80	0.00	270.03
95-a1	2.40	114.24	40.32	14.40	7.68	15.84	11.28	4.32	4.56	2.64	0.41	0.55	0.02	15.84	5.76	237.86
95-a2	2.50	132.00	29.00	10.75	16.00	27.25	15.75	5.00	4.00	3.25	0.28	0.47	0.03	5.50	2.75	252.02
95-a3	2.80	152.60	45.64	7.28	12.88	24.36	23.52	8.96	3.36	2.30	0.70	0.36	0.06	1.18	0.84	284.03

File name: wtci1

WEIGHTS ASSUMING TiO2 CONSTANT																
Sample	TiR	SiO2	Al2O3	Fe2O3	FeO	MgO	CaO	Na2O	K2O	TiO2	P2O5	MnO	CO2	H2O+	H2O-	Sum
109-a1	0.46	16.32	8.07	7.33	2.02	1.28	1.47	0.14	0.23	2.20	0.18	0.09	0.05	4.35	1.56	45.28
109-a2	0.56	21.44	6.77	11.85	0.00	2.99	4.06	0.57	0.46	2.20	0.00	0.10	0.00	6.04	0.00	56.41
109-a3	0.71	29.10	8.52	12.77	0.00	3.76	5.89	1.31	0.57	2.20	0.00	0.14	0.00	6.74	0.00	70.97
109-a4	1.00	53.70	14.10	1.90	9.80	4.20	8.10	2.80	1.50	2.20	0.40	0.20	0.10	1.20	0.30	100.50
105-a1	1.05	56.28	17.64	7.35	3.15	2.83	5.67	2.31	1.15	2.10	0.32	0.21	0.10	4.31	1.89	105.31
105-a2	1.00	53.40	15.00	2.00	9.00	4.20	8.10	2.80	1.30	2.10	0.40	0.20	0.10	1.20	0.50	100.30
104-a1	0.71	30.92	8.12	3.11	10.45	6.00	4.52	1.48	0.49	2.40	0.21	0.14	0.07	1.76	0.21	70.24
104-a2	0.77	33.99	9.21	2.48	11.85	6.74	6.12	1.86	0.39	2.40	0.31	0.15	0.08	0.85	0.08	76.49
104-a3	1.00	46.50	15.80	2.00	2.10	6.90	9.10	3.00	0.50	2.40	0.30	0.20	0.10	0.50	0.20	99.60
102-a1	0.58	20.84	5.56	13.52	0.00	3.71	3.82	0.56	0.43	2.20	0.00	0.15	0.00	7.29	0.00	57.89
102-a2	0.69	27.50	7.56	13.75	0.00	4.16	5.29	1.21	0.51	2.20	0.00	0.17	0.00	6.39	0.00	68.75
102-a3	1.00	48.00	14.00	14.00	0.00	4.18	8.50	3.05	0.96	2.20	0.00	0.19	0.00	5.00	0.00	100.00
98-a1	0.73	33.53	9.60	4.00	7.64	4.73	5.75	1.67	0.51	2.40	0.22	0.15	0.07	1.38	0.07	71.71
98-a2	1.00	48.80	15.90	4.00	9.90	6.50	9.20	2.90	0.50	2.40	0.30	0.20	0.10	0.40	0.10	101.20

File name: nwtci1

NORMALIZED WEIGHTS ASSUMING TiO2 CONSTANT																
Sample	TiR	SiO2	Al2O3	Fe2O3	FeO	MgO	CaO	Na2O	K2O	TiO2	P2O5	MnO	CO2	H2O+	H2O-	Sum
109-a1	0.46	0.30	0.57	3.86	0.21	0.31	0.18	0.05	0.15	1.00	0.46	0.46	0.46	3.63	5.19	0.45
109-a2	0.56	0.40	0.48	6.23	0.00	0.71	0.50	0.20	0.30	1.00	0.00	0.51	0.00	5.03	0.00	0.56
109-a3	0.71	0.54	0.60	6.72	0.00	0.90	0.73	0.47	0.38	1.00	0.00	0.71	0.00	5.62	0.00	0.71
109-a4	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
105-a1	1.05	1.05	1.18	3.67	0.35	0.67	0.70	0.82	0.89	1.00	0.79	1.05	1.05	3.59	3.78	1.05
105-a2	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
104-a1	0.71	0.66	0.51	1.55	4.97	0.87	0.50	0.49	0.99	1.00	0.71	0.71	0.71	3.53	1.06	0.71
104-a2	0.77	0.73	0.58	1.24	5.64	0.98	0.67	0.62	0.77	1.00	1.03	0.77	0.77	1.70	0.39	0.77
104-a3	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
102-a1	0.58	0.43	0.40	0.95	0.00	0.89	0.45	0.18	0.45	1.00	0.00	0.79	0.00	1.46	0.00	0.58
102-a2	0.69	0.57	0.54	0.98	0.00	1.00	0.62	0.40	0.53	1.00	0.00	0.87	0.00	1.28	0.00	0.69
102-a3	1.00	1.00	1.00	1.00	0.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00
98-a1	0.73	0.69	0.60	1.00	0.77	0.73	0.62	0.58	1.02	1.00	0.73	0.73	0.73	3.45	0.73	0.71
98-a2	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00