UNITED STATES DEPARTMENT OF THE INTERIOR

GEOLOGICAL SURVEY

CHEMANAL: A MULTICS Fortran program to calculate chemical weathering data

by

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Open-File Report 80-844

1980

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	SiO2	"
5	Al2O3	"
6	Fe2O3	"
7	FeO	"
8	MgO	"
9	CaO	"
10	Na2O	"
11	K2O	"
12	TiO2	"
13	P2O5	"
14	MnO	"
15	CO2	"
16	H2O+	"
17	H2O-	"
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, Graphi 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 catios? (0=no,1=yes)
? 1
Output file name for standard cell catios?
? 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 (sam
ples)? (0=no, 1=yes)
? 0

STOP
```

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.

```
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                    *                              *
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,16)=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 R203
      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 SiO2/R203
      xmpr(k,8) = xmpc(k,3)/xmpr(k,4)
c bases/R203
      xmpr(k,9) = xmpr(k,3)/xmpr(k,4)
c Fe203:FeO
      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 SiO2-R203-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 (xmpr(mm,j)) 812,813,812
813   xnmpr(k,j)=0.0
      go to 803
```

```
812     xnmpr(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:R2 Fe3Fe2  TriSi  TriR2 TriBas")
        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
      tsso(k,1) = tmpc(k,1)*2.0/tmpc(k,14)
      tssi(k,1) =  tmpc(k,1)/tmpc(k,14)
c Al
      tsso(k,2) = (tmpc(k,2)*3)/tmpc(k,14)
      tssi(k,2) = (tmpc(k,2)*2)/tmpc(k,14)
c Fe3
      tsso(k,3) = (tmpc(k,3)*3)/tmpc(k,14)
      tssi(k,3) = (tmpc(k,3)*2)/tmpc(k,14)
c Fe2
      tsso(k,4) = (tmpc(k,4))/tmpc(k,14)
      tssi(k,4) = (tmpc(k,4))/tmpc(k,14)
c Mg
      tsso(k,5) = tmpc(k,5)/tmpc(k,14)
      tssi(k,5) = tmpc(k,5)/tmpc(k,14)
c Ca
      tsso(k,6) = tmpc(k,6)/tmpc(k,14)
      tssi(k,6) = tmpc(k,6)/tmpc(k,14)
c Na
      tsso(k,7) = tmpc(k,7)/tmpc(k,14)
      tssi(k,7) = tmpc(k,7)*2.0/tmpc(k,14)
c K
      tsso(k,8) = tmpc(k,8)/tmpc(k,14)
      tssi(k,8) = tmpc(k,8)*2.0/tmpc(k,14)
c Ti
      tsso(k,9) = tmpc(k,9)*2.0/tmpc(k,14)
      tssi(k,9) = tmpc(k,9)/tmpc(k,14)
c P
      tsso(k,10) = (tmpc(k,10)*5)/tmpc(k,14)
      tssi(k,10) = (tmpc(k,10)*2)/tmpc(k,14)
c Mn
      tsso(k,11) = tmpc(k,11)/tmpc(k,14)
      tssi(k,11) = tmpc(k,11)/tmpc(k,14)
c C
      tsso(k,12) = tmpc(k,12)*2.0/tmpc(k,14)
      tssi(k,12) = tmpc(k,12)/tmpc(k,14)
c H
      tsso(k,13) = tmpc(k,13)/tmpc(k,14)
      tssi(k,13) = tmpc(k,13)*2.0/tmpc(k,14)
c Sum of O
      tot=0.0
      do 204 j=1,13
      tot = tot + tsso(k,j)
204   continue
      tsso(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    Ti    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
     cO  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)
64    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                  *     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	0.5	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	0.0-2.6	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	0.30	0.20	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	R2O3	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	3.64	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	73.38	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: nmr1

NORMALIZED MOLECULAR RATIOS

Sample	Bases	R2O3	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	1.31	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 CATIONS

Sample	Si	Al	Fe3+	Fe2+	Mg	Ca	Na	K	Ti	P	Mn	C	H	Sum
109-a1	33.04	19.22	11.16	3.41	3.87	3.18	0.54	0.59	3.37	0.31	0.16	0.13	58.77	137.75
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	36.63	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	3.62	5.21	3.83	1.26	1.36	0.23	0.15	0.12	24.62	113.48
105-a2	50.26	16.61	1.42	7.08	5.89	8.17	5.10	1.56	1.50	0.32	0.16	0.13	7.53	105.72
104-a1	43.32	13.38	3.27	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	11.67	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	5.67	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	2.68	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 CATIONS

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	BD	SiO2	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	256.68
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	2.80	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	BD	SiO2	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: wtc1

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	13.32	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: nwtc1

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