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1985/12. CHEMFORM: A FORTRAN program for calculating the chemical formula of a mineral from its analysis

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Abstract

CHEMFORM is a Fortran program for calculating the chemical formula of a mineral from its analysis.

INTRODUCTION

The program CHEMFORM is written in FORTRAN 77 and runs interactively on the Department of Mines Perkin-Elmer 8/32 mini-computer. The input is the weight percent of any or all of the oxides SiO_2 , TiO_2 , Al_2O_3 , Cr_2O_3 , FeO , MnO , MgO , CaO and Na_2O . The output is a structural formula based on the specified number of oxygen atoms. The ratios of $\text{Mg}:(\text{Mg}+\text{Fe})$, $\text{Ca}:(\text{Ca}+\text{Mg}+\text{Fe})$, $\text{Mg}:(\text{Ca}+\text{Mg}+\text{Fe})$, $\text{Fe}:(\text{Ca}+\text{Mg}+\text{Fe})$ and $\text{Cr}:(\text{Cr}+\text{Al})$ are also calculated and tabulated.

RUNNING THE PROGRAM

To run the program type "CHEMFORM" and supply the answers to the screen prompts. It will be necessary to enter sample identification (up to 12 characters) followed by the weight percent of each of the oxides. If the analysis indicates that a particular oxide was absent, then enter zero in response to the prompt for that oxide. If you realise that you have entered a weight percent incorrectly and wish to start again then enter any character in response to the next weight percent prompt. The program will then start again at the beginning with the prompt for sample identification. This is illustrated in the sample run (Appendix 1) where the weight percent for TiO_2 was incorrectly entered and the entering of data is recommenced by typing any character ("D" in this example) in response to the next weight percent prompt. Following the entry of the weight percent data the number of oxygen atoms must be entered. The program then has the required information to carry out the calculations. In the second example of Appendix 2 Al_2O_3 and Cr_2O_3 were absent and thus the ratio $\text{Cr}:(\text{Cr}+\text{Al})$ has no meaning. In such a case the program will output four asterisks as the ratio. This may be seen in Appendix 2 which is the printed output obtained from the interactive session shown in Appendix 1.

PROGRAM LISTING

The program is listed in Appendix 3.

[21 March 1985]

APPENDIX 1

Log of sample session

CHEMFORM

ENTER SAMPLE IDENTIFICATION
C147-OL
ENTER WEIGHT PERCENT OF SiO2
40.85
ENTER WEIGHT PERCENT OF TiO2
6.51
ENTER WEIGHT PERCENT OF Al2O3

D
ENTER SAMPLE IDENTIFICATION
C147-OL
ENTER WEIGHT PERCENT OF SiO2
40.85
ENTER WEIGHT PERCENT OF TiO2
0.0
ENTER WEIGHT PERCENT OF Al2O3
0.0
ENTER WEIGHT PERCENT OF Cr2O3
0.0
ENTER WEIGHT PERCENT OF FeO
6.51
ENTER WEIGHT PERCENT OF MnO
0.0
ENTER WEIGHT PERCENT OF MgO
52.44
ENTER WEIGHT PERCENT OF CaO
0.0
ENTER WEIGHT PERCENT OF Na2O
0.0
TOTAL IS 99.80
ENTER NO. OF OXYGEN ATOMS

4
AGAIN? (N/Y)

Y
ENTER SAMPLE IDENTIFICATION
C147-SP
ENTER WEIGHT PERCENT OF SiO2
0.0
ENTER WEIGHT PERCENT OF TiO2
0.0
ENTER WEIGHT PERCENT OF Al2O3
4.23
ENTER WEIGHT PERCENT OF Cr2O3
65.23
ENTER WEIGHT PERCENT OF FeO
23.91
ENTER WEIGHT PERCENT OF MnO
0.0
ENTER WEIGHT PERCENT OF MgO
6.12
ENTER WEIGHT PERCENT OF CaO
0.0
ENTER WEIGHT PERCENT OF Na2O
0.0
TOTAL IS 99.49
ENTER NO. OF OXYGEN ATOMS

32
AGAIN? (N/Y)

N
J -END OF TASK CODE= 0 PROCESSOR=0.374 TSK-ELAPSED=2:11

APPENDIX 2

Printed output from sample session of Appendix 1

SAMPLE - C147-OL

NO. OF OXYGEN ATOMS - 4

	wt.% of oxides	atom.props. of oxygen	Nos. of anions (4 O basis)	Nos. of ions in formula
SiO2	40.85	1.3596	1.977	Si 0.9885
TiO2	0.00	0.0000	0.000	Ti 0.0000
Al2O3	0.00	0.0000	0.000	Al 0.0000
Cr2O3	0.00	0.0000	0.000	Cr 0.0000
FeO	6.51	0.0906	0.132	Fe 0.1318
MnO	0.00	0.0000	0.000	Mn 0.0000
MgO	52.44	1.3006	1.891	Mg 1.8912
CaO	0.00	0.0000	0.000	Ca 0.0000
Na2O	0.00	0.0000	0.000	Na 0.0000
TOTAL	99.80	2.7508		3.0115

Mg/(Mg+Fe)=93.5%
 Ca/(Ca+Mg+Fe)= 0.0%; Mg/(Ca+Mg+Fe)=93.5%; Fe/(Ca+Mg+Fe)= 6.5%
 Cr/(Cr+Al)=****%

SAMPLE - C147-SP

NO. OF OXYGEN ATOMS - 32

	wt.% of oxides	atom.props. of oxygen	Nos. of anions (32 O basis)	Nos. of ions in formula
SiO2	0.00	0.0000	0.000	Si 0.0000
TiO2	0.00	0.0000	0.000	Ti 0.0000
Al2O3	4.23	0.1245	2.101	Al 1.4004
Cr2O3	65.23	1.2873	21.722	Cr 14.4816
FeO	23.91	0.3328	5.616	Fe 5.6156
MnO	0.00	0.0000	0.000	Mn 0.0000
MgO	6.12	0.1518	2.561	Mg 2.5614
CaO	0.00	0.0000	0.000	Ca 0.0000
Na2O	0.00	0.0000	0.000	Na 0.0000
TOTAL	99.49	1.8963		24.0590

Mg/(Mg+Fe)=31.3%
 Ca/(Ca+Mg+Fe)= 0.0%; Mg/(Ca+Mg+Fe)=31.3%; Fe/(Ca+Mg+Fe)=68.7%
 Cr/(Cr+Al)=91.2%

APPENDIX 3

CHEMFORM Program Listing

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C * * * * *
  REAL X(10),Y(10),Z(10),S(10),RAT(5)
  INTEGER OXNO
  CHARACTER*12 SAMP
  CHARACTER*5 ELEM(9)
  CHARACTER*1 ANS
  DATA ELEM /'SiO2 ','TiO2 ','Al2O3','Cr2O3','FeO ','MnO ','
1'MgO ','CaO ','Na2O '/
15 SAMP='
   Z(10)=0.0
   Y(10)=0.0
   X(10)=0.0
   S(10)=0.0
   WRITE(5,20)
20 FORMAT(1X,'ENTER SAMPLE IDENTIFICATION')
   READ(5,25) SAMP
25 FORMAT(A12)
   DO 100 J=1,9
   WRITE(5,40) ELEM(J)
40 FORMAT(1X,'ENTER WEIGHT PERCENT OF ',A5)
   READ(5,*,ERR=15) Z(J)
   Z(10)=Z(10)+Z(J)
100 CONTINUE
   WRITE(5,110) Z(10)
110 FORMAT(1X,'TOTAL IS',F7.2)
C * * * * *
  X(1)=2*Z(1)/60.09
  X(2)=2*Z(2)/79.90
  X(3)=3*Z(3)/101.94
  X(4)=3*Z(4)/152.02
  X(5)=Z(5)/71.85
  X(6)=Z(6)/70.94
  X(7)=Z(7)/40.32
  X(8)=Z(8)/56.08
  X(9)=Z(9)/61.982
  DO 120 J=1,9
  X(10)=X(10)+X(J)
120 CONTINUE
   WRITE(5,125)
125 FORMAT(1X,'ENTER NO. OF OXYGEN ATOMS')
   READ(5,*) OXNO
   FACT=OXNO/X(10)
   DO 200 J=1,9
   Y(J)=FACT*X(J)
200 CONTINUE
   S(1)=Y(1)*0.5
   S(2)=Y(2)*0.5
   S(3)=Y(3)*(2.0/3.0)
   S(4)=Y(4)*(2.0/3.0)
   DO 240 J=5,8
   S(J)=Y(J)
240 CONTINUE
   S(9)=Y(9)*2.0
   DO 270 J=1,9
   S(10)=S(10)+S(J)

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270 CONTINUE
    WRITE(6,280) SAMP,OXNO,OXNO
280 FORMAT(//////,1X,'SAMPLE - ',A12,/,1X,'NO. OF OXYGEN ATOMS - ',
1I3,/,15X,'wt.% of',6X,'atom.props.',3X,'Nos.of anions',2X,
2'Nos. of ions',/,15X,'oxides',8X,'of oxygen',4X,'(',I2,
3' 0 basis)',4x,'in formula')
    DO 350 J=1,9
    WRITE(6,340) ELEM(J),Z(J),X(J),Y(J),ELEM(J)(1:2),S(J)
340 FORMAT(1X,A5,F15.2,F15.4,F15.3,6X,A2,F9.4)
350 CONTINUE
    WRITE(6,365) Z(10),X(10),S(10)
365 FORMAT(16X,'-----',9X,'-----',25X,'-----',
1/,1X,'TOTAL',9X,F6.2,8X,F7.4,23X,F9.4,/,16X,'-----',
29X,'-----',25X,'-----')
    IF(S(5).EQ.0.AND.S(7).EQ.0) THEN
    RAT(1)=1000000.0
    ELSE
    RAT(1)=100.0*S(7)/(S(5)+S(7))
    ENDIF
    IF(S(5).EQ.0.0.AND.S(7).EQ.0.0.AND.S(8).EQ.0.0) THEN
    RAT(2)=10000000.0
    RAT(3)=10000000.0
    RAT(4)=10000000.0
    ELSE
    RATDEN=0.01*(S(5)+S(7)+S(8))
    RAT(2)=S(8)/RATDEN
    RAT(3)=S(7)/RATDEN
    RAT(4)=S(5)/RATDEN
    ENDIF
    IF(S(3).EQ.0.0.AND.S(4).EQ.0.0) THEN
    RAT(5)=10000000.0
    ELSE
    RAT(5)=100.0*S(4)/(S(4)+S(3))
    ENDIF
    WRITE(6,370) RAT
370 FORMAT(1X,67(' '),/,1X,'Mg/(Mg+Fe)=' ,F4.1,'%',/,1X,
1'Ca/(Ca+Mg+Fe)=' ,F4.1,'%', Mg/(Ca+Mg+Fe)=' ,F4.1,
2'%', Fe/(Ca+Mg+Fe)=' ,F4.1,'%',/,1X,'Cr/(Cr+Al)=' ,F4.1,'%')
    WRITE(5,610)
610 FORMAT(1X,'AGAIN? (N/Y)')
612 READ(5,613) ANS
613 FORMAT(A1)
    IF(ANS.EQ.'Y') GO TO 15
    IF(ANS.NE.'N') THEN
    WRITE(5,618)
618 FORMAT(1X,'ANSWER N OR Y')
    GO TO 612
    ENDIF
    WRITE(6,710)
710 FORMAT(1X)
    END

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