JOURNAL OF ELECTRON MICROSCOPY TECHNIQUE 2:637–642 (1985)

A FORTRAN Computer Program for Converting Among Atom, Weight, and Oxide Percentages for Use in Analytical Electron Microscopy

W.C. BIGELOW
Department of Materials and Metallurgical Engineering, University of Michigan, Ann Arbor, Michigan 48109

KEY WORDS Computer program chemical formula calculations, oxide percent calculations

ABSTRACT A FORTRAN program is given which will (1) calculate atom and weight percentages from a given chemical formula: (2) calculate atom percentages from given weight percentages; (3) calculate oxide percentages from given weight percentages; and (4) calculate weight percentages from given oxide percentages. The program is interactive, easy to use, and very convenient for use in electron beam microanalytical work.

INTRODUCTION

Many scanning electron microscopes are now equipped with either energy-dispersive or crystal spectrometer systems capable of carrying out quantitative chemical analyses. When working with such systems it is frequently desirable to make conversions among weight, atom, and oxide percentages. This is particularly true when dealing with ceramic, mineral, and intermetallic phases. Such conversions are tedious to perform by hand, and most computer-based analytic systems do not provide a program for carrying them out.

The program CCC (Chemical Composition Converter) listed here allows the following conversions to be carried out in a straightforward manner for phases containing up to 15 elements:

(1) conversion from chemical formula to atomic and weight percent,

(2) conversion from atom percent to weight percent,

(3) conversion from weight percent to oxide percent, and

(4) conversion from oxide percent to weight percent.

The program is written in FORTRAN, but is organized so that it should be easily translated into BASIC. Each of the above conversion processes is handled in a separate subroutine so any not needed in a particular laboratory can be omitted. The subroutine for conversion from chemical formula to atomic and weight percentages will accept noninteger coefficients to facilitate calculations for phases involving chemical substitution. This is illustrated in the examples of the program's output shown below.

EXAMPLES OF CALCULATIONS USING THE PROGRAM CCC
FOR THE MINERAL $Na_{.1}K_{.9}AlSi_3O_8$

CALCULATE ATOM AND WEIGHT PERCENTS FROM CHEMICAL FORMULA

ELMT	ATNO	ATMC WT	#/MOL	AT PCT	WT PCT	EL
NA	11	22.990	0.10	0.769	0.831	NA
K	19	39.102	0.90	6.923	12.717	K
AL	13	26.982	1.00	7.692	9.751	AL
SI	14	28.086	3.00	23.077	30.449	SI
O	8	15.999	8.00	61.538	46.253	O

Received January 10, 1985; accepted March 24, 1985.

Address reprint requests to W.C. Bigelow, Dept. of Materials and Metallurgical Engineering, Dow Building, 1500 Hayward Street, University of Michigan, Ann Arbor, MI 48109.

CALCULATE OXIDE PERCENT FROM WEIGHT PERCENT

ELMT	ATNO	ATOM WT	WT PCT	OXIDE	OX PCT	EL
NA	11	22.990	0.831	NA201	1.120	NA
K	19	39.102	12.717	K 201	15.319	K
AL	13	26.982	9.751	AL203	18.424	AL
SI	14	28.086	30.449	SI102	65.139	SI
WT PCT OXYGEN= 46.253				TOTAL= 100.002		

CALCULATE WEIGHT PERCENT FROM OXIDE PERCENT

ELMT	ATNO	ATMC WT	OXIDE	OX PCT	WT PCT	EL
NA	11	22.990	NA201	1.120	0.831	NA
K	19	39.102	K 201	15.319	12.717	K
AL	13	26.982	AL203	18.424	9.751	AL
SI	14	28.086	SI102	65.139	30.449	SI
WT PCT OXYGEN= 46.254				TOTAL= 100.002		

CALCULATE ATOM PERCENT FROM WEIGHT PERCENT

ELMT	ATNO	ATMC WT	WT PCT	AT PCT	EL
NA	11	22.990	0.831	0.769	NA
K	19	39.102	12.717	6.923	K
AL	13	26.982	9.751	7.693	AL
SI	14	28.086	30.449	23.077	SI
O	8	15.999	46.253	61.538	O
TOTALS:			100.001	100.000	

```
C       SOURCE.CCC
CCC   PROGRAM TO CONVERT AMONG WT, ATM, & OXIDE PCTS.
C     W. C. BIGELOW, UNIVERSITY OF MICHIGAN
C
      WRITE(5,11)
   11 FORMAT(2X/,6X,'CCC, A PROG TO CONVERT AMONG WT,'
     @' ATOM AND OXIDE PCTS')
   10 WRITE(5,1)
    1 FORMAT(2X/6X,'DO YOU WANT TO CALCULATE:'/9X,
     @'1=WT & ATM PCTS FROM CHEM FORMULA '/9X,
     @'2=WT PCT FROM OXIDE PCT '/9X,
     @'3=OXIDE PCT FROM WT PCT CATIONS'/9X,
     @'4=ATOM PCT FROM WT PCT '/9X,
     @'PRESS RETURN KEY TO STOP'/2X/6X,
     @'TYPE NO. OF CHOICE',$)
C
      READ(5,2)N
    2 FORMAT(I1)
      GOTO(70,20,30,40,50)N+1
      GOTO 10
   20 CALL WTCH
      GOTO 10
   30 CALL WTOX
      GOTO 10
   40 CALL OXWT
      GOTO 10
   50 CALL ATWT
      GOTO 10
   70 CONTINUE
      END
```

```
C       SOURCE ATWTNO
CCC    SUB TO GET AT NO & AT WT FROM AT SYM
C      FOR USE WITH PROG CCC
C      W. C. BIGELOW, UNIVERSITY OF MICHIGAN
C
       SUBROUTINE ATWTNO(ASYM,XWT,NATM)
       DIMENSION ATWT(92),ATSYM(92)
       DATA ATSYM/'H ','HE','LI','BE','B ','C ','N ','O ',
      @'F ','NE','NA','MG','AL','SI','P ','S ','CL','AR','K ',
      @'CA','SC','TI','V ','CR','MN','FE','CO','NI','CU','ZN',
      @'GA','GE','AS','SE','BR','KR','RB','SR','Y ','ZR','NB',
      @'MO','TC','RU','RH','PD','AG','CD','IN','SN','SB','TE',
      @'I ','XE','CS','BA','LA','CE','PR','ND','PM','SM','EU',
      @'GD','TB','DY','HO','ER','TM','YB','LU','HF','TA','W ',
      @'RE','OS','IR','PT','AU','HG','TL','PB','BI','PO','AT',
      @'RN','FR','RA','AC','TH','PA','U '/
       DATA ATWT/1.008,4.003,6.939,9.012,10.811,12.011,
      @14.007,15.999,18.998,20.183,22.990,24.312,26.982,
      @28.086,30.974,32.064,35.453,39.948,39.102,40.080,
      @44.956,47.90,50.942,51.996,54.938,55.847,58.933,58.71,
      @63.54,63.37,69.72,72.59,74.922,78.96,79.909,83.80,
      @85.47,87.62,88.905,91.22,92.906,95.94,99.0,101.07,
      @102.905,106.4,107.870,112.40,114.82,118.69,121.75,
      @127.60,126.904,131.30,132.905,137.34,138.91,140.12,
      @140.907,144.24,145.,150.35,151.96,157.25,158.924,
      @162.50,164.930,167.26,168.934,173.04,174.97,178.49,
      @180.948,183.85,186.2,190.2,192.2,195.09,196.967,
      @200.59,204.37,207.19,208.980,210.0,210.0,222.,223.,227.,
      @227.,232.038,231.0,238.03/
       DATA BLNK/'  '/
     3 DO 5 I=1,92
       IF(ASYM.NE.ATSYM(I))GOTO 5
       NATM=I
       XWT=ATWT(I)
       RETURN
     5 CONTINUE
       WRITE(5,7)ASYM
     7 FORMAT(2X/6X,'CANT FIND ATM SYM:  ',A2/2X/
      @6X,'WRITE CORRECT SYMBOL: ',$)
       READ(5,8)ASYM
       IF(ASYM.EQ.BLNK)GOTO 9
       GOTO 3
     9 WRITE(5,10)
    10 FORMAT(2X/6X,'*** NO ELMT GIVEN - CALCS END')
       STOP
     8 FORMAT(A2)
       END
>
```

```
C       SOURCE.ATWT
C      SUB TO CONVERT FROM WT PCT TO ATM PCT
C      FOR USE WITH PROG CCC
C        W.C. BIGELOW.  UNIVERSITY OF MICHIGAN
C
       SUBROUTINE ATWT
       COMMON /CBL/SYM(15),AWT(15),NZ(15),ELPCT(15)
       DATA BLNK/'  '/
     1 DO 15 I=1,15
       WRITE(5,3)I
     3 FORMAT(2X/6X,'SYMBOL FOR ELMT NO. ',I2,': ',$)
       READ(5,4)SYM(I)
     4 FORMAT(A2)
       IF(SYM(I).NE.BLNK)GOTO 6
       JNUM=I-1
       GOTO 19
     6 ASYM=SYM(I)
       CALL ATWTNO(ASYM,XWT,NATM)
       AWT(I)=XWT
       NZ(I)=NATM
```

```
      WRITE(5,8)
    8 FORMAT(6X,'WT PCT THIS ELEMT ',$)
      READ(5,9)ELPCT(I)
    9 FORMAT(F8.0)
   15 CONTINUE
C
   19 WRITE(6,20)
   20 FORMAT(2X/2X/7X,'ELMT',1X,'ATNO',1X,'ATMC WT',2X,
     @'WT PCT',2X,'AT PCT',2X,'EL')
C
      SUM=0.0
   21 DO 22 J=1,JNUM
   22 SUM=SUM+(ELPCT(J)/AWT(J))
      WTOT=0.0
      ATOT=0.0
      DO 28 J=1,JNUM
      ATPCT=(100.0*ELPCT(J)/AWT(J))/SUM
      ATOT=ATOT+ATPCT
      WTOT=WTOT+ELPCT(J)
C
      WRITE(6,25)SYM(J),NZ(J),AWT(J),ELPCT(J),ATPCT,SYM(J)
   25 FORMAT(8X,A2,3X,I2,2X,F7.3,2X,F6.3,2X,F6.3,2X,A2)
   28 CONTINUE
      WRITE(6,31)WTOT,ATOT
   31 FORMAT(10X,'TOTALS:',8X,F7.3,1X,
     @F7.3/2X/2X/2X)
      ENDFILE 6
      RETURN
      END
>
```

```
C     SOURCE OXWT
C     SUB TO CONVERT FROM OXIDE TO WT PCT
C     FOR USE WITH PROG CCC
C     W. C. BIGELOW. UNIVERSITY OF MICHIGAN
C
      SUBROUTINE OXWT
      COMMON /CBL/SYM(15),AWT(15),NZ(15),ELPCT(15)
     @/CBM/NEL(15),NOX(15)
      DATA BLNK/'  '/
    1 DO 15 I=1,15
      WRITE(5,3)I
    3 FORMAT(2X/6X,'SYM FOR ELMT NO. ',I2,':',$)
      READ(5,4)SYM(I)
    4 FORMAT(A2)
      IF(SYM(I).NE.BLNK)GOTO 6
      JNUM=I-1
      GOTO 19
    6 WRITE(5,7)
    7 FORMAT(6X,'WT PCT OF THIS ELMT: ',$)
      READ(5,8)ELPCT(I)
    8 FORMAT(F8.0)
      WRITE(5,9)
    9 FORMAT(6X,'NO. ATOMS THIS ELMT IN ITS OXIDE: ',$)
      READ(5,10)NEL(I)
   10 FORMAT(I2)
      WRITE(5,12)
   12 FORMAT(/,6X,'NO. OXYGEN ATOMS IN ITS OXIDE: ',$)
      READ(5,10)NOX(I)
      ASYM=SYM(I)
      CALL ATWINO(ASYM,XWT,NATM)
      AWT(I)=XWT
      NZ(I)=NATM
   15 CONTINUE
   19 WRITE(6,20)
   20 FORMAT(2X/2X/7X,'ELMT',1X,'ATNO',1X,'ATOM WT',2X,
     @'WT PCT',2X,'OXIDE',2X,'OX PCT',2X,'EL')
      TOX=0.0
```

```
      TPCT=0.0
      DO 22 J=1,JNUM
      WTOX=(ELPCT(J)*NOX(J)*15.999)/(AWT(J)*NEL(J))
      OXPCT=WTOX+ELPCT(J)
      TPCT=TPCT+OXPCT
      TOX=TOX+WTOX
      WRITE(6,21)SYM(J),NZ(J),AWT(J),ELPCT(J),SYM(J),NEL(J),
     @NOX(J),OXPCT,SYM(J)
   21 FORMAT(8X,A2,3X,I2,2X,F7.3,2X,F6.3,2X,A2,I1,'O',
     @I1,2X,F6.3,2X,A2)
   22 CONTINUE
      TOX=TOX*100./TPCT
      WRITE(6,23)TOX,TPCT
   23 FORMAT(10X,'WT PCT OXYGEN=',F7.3,2X,'TOTAL= ',
     @F7.3/2X/2X/2X)
      ENDFILE 6
      RETURN
      END
```

```
C       SOURCE WTCH
CCC    SUB TO CALC WT PCT FROM CHEM FORMULA
C      FOR USE WITH PROG CCC
C      W. C. BIGELOW, UNIVERSITY OF MICHIGAN
C
       SUBROUTINE WTCH
       DATA SP/'  '/
       COMMON /CBL/SYM(15),AWT(15),NZ(15),ATMS(15)
       DO 15 I=1,15
       WRITE(5,8)I
     8 FORMAT(2X/6X,'SYM FOR ELMT NO. ',I1,': ',$)
       READ(5,9)ASYM
     9 FORMAT(A2)
       IF(ASYM.EQ.SP)GOTO 16
       SYM(I)=ASYM
       CALL ATWTNO(ASYM,XWT,NATM)
       AWT(I)=XWT
       NZ(I)=NATM
    13 WRITE(5,10)
    10 FORMAT(5X,'NO. ATOMS OF THIS ELMT IN FORMULA: ',$)
       READ(5,11)ATMS(I)
    11 FORMAT(F8.0)
    15 CONTINUE
    16 NELS=I-1
       WRITE(6,17)
    17 FORMAT(2X/2X/7X,'ELMT',1X,'ATNO',1X,'ATMC WT',2X,
      @'#/MOL',2X,'AT PCT',2X,'WT PCT',2X,'EL')
       WSUM=0.0
       ASUM=0.0
       DO 18 I=1,NELS
       ASUM=ASUM+ATMS(I)
    18 WSUM=WSUM+(AWT(I)*ATMS(I))
       DO 20 J=1,NELS
       APCT=ATMS(J)*100.0/ASUM
       WPCT=AWT(J)*ATMS(J)*100.0/WSUM
       WRITE(6,19)SYM(J),NZ(J),AWT(J),ATMS(J),APCT,WPCT,SYM(J)
    19 FORMAT(8X,A2,3X,I2,2X,F7.3,2X,F5.2,2X,F6.3,2X,F6.3,2X,A2)
    20 CONTINUE
C
       WRITE(6,22)
    22 FORMAT(2X/2X/2X)
       ENDFILE 6
       RETURN
       END
>
```

```
C       SOURCE  WTOX
C      SUBROUTINE TO CONVERT FROM OXIDE TO WT PCT
C      FOR USE WITH PROG CCC
C       W. C. BIGELOW,  UNIVERSITY OF MICHIGAN
C
       SUBROUTINE WTOX
       COMMON /CBL/SYM(15),AWT(15),NZ(15),OXPCT(15)
      @/CBM/NEL(15),NOX(15)
       DATA BLNK/' '/
     1 DO 15 I=1,15
       WRITE(5,2)I
     2 FORMAT(2X/6X,'NO. OF OXYGEN ATOMS IN OXIDE NO. ',I2,': ',$)
       READ(5,4)NOX(I)
     4 FORMAT(I1)
       IF(NOX(I).NE.0)GOTO 5
     7 JNUM=I-1
       IF(JNUM.LT.2)GOTO 28
       GOTO 19
     5 WRITE(5,6)
     6 FORMAT(6X,'SYM OF OTHER ELMT IN THIS OXIDE: ',$)
       READ(5,8)SYM(I)
     8 FORMAT(A2)
       WRITE(5,10)
    10 FORMAT(6X,'NO. OF ATOMS OF THIS ELMT: ',$)
       READ(5,4)NEL(I)
       IF(NEL(I).LT.1)GOTO 7
       ASYM=SYM(I)
       CALL ATWTNO(ASYM,XWT,NATM)
       AWT(I)=XWT
       NZ(I)=NATM
       WRITE(5,12)
    12 FORMAT(/,6X,'OXIDE PCT OF THIS OXIDE: ',$)
       READ(5,13)OXPCT(I)
    13 FORMAT(F8.0)
    15 CONTINUE
C
    19 WRITE(6,20)
    20 FORMAT(2X/2X/7X,'ELMT',1X,'ATNO',1X,'ATMC WT',2X,
      @'OXIDE',2X,'OX PCT',2X,'WT PCT',2X,'EL')
C
       TPCT=0.0
       PCTOX=0.0
       DO 23 J=1,JNUM
       SUM=NOX(J)*15.999+NEL(J)*AWT(J)
       WPCT=NEL(J)*AWT(J)*OXPCT(J)/SUM
       PCTOX=PCTOX+(NOX(J)*15.999*OXPCT(J)/SUM)
       TPCT=TPCT+WPCT
       WRITE(6,22)SYM(J),NZ(J),AWT(J),SYM(J),NEL(J),
      @NOX(J),OXPCT(J),WPCT,SYM(J)
    22 FORMAT(8X,A2,3X,I2,2X,F7.3,2X,A2,I1,'O',I1,2X,
      @F6.3,2X,F6.3,2X,A2)
    23 CONTINUE
       TPCT=TPCT+PCTOX
       WRITE(6,25)PCTOX,TPCT
    25 FORMAT(9X,'WT PCT OXYGEN=',F7.3,3X,'TOTAL= ',F7.3,
      @2X/2X/2X/2X)
       ENDFILE 6
       RETURN
    28 WRITE(5,29)
    29 FORMAT(/6X,'LESS THAN 2 OXIDES - USE CHEM FORMULA')
       RETURN
       END
>
```