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A Fortran Version of the Quantitative Energy-Dispersive Electron Beam X-ray Analysis Program FRAME C

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Foreword

This publication was written as a supplement to NBS Technical Note 1106 entitled FRAME C: A Compact Procedure for Quantitative Energy- Dispersive Electron Probe X-ray Analysis. The original publication documented a BASIC language computer program for on-line use with a multi-channel analyzer. This publication documents a FORTRAN version of a similar program. The description of the quantitative analysis procedure is not reproduced in this publication. Readers should consult NBS Technical Note 1106 for this description. Together with the documented program listing, a description of the input and output of the program is presented, as well as an example.

The program is written in FORTRAN 77 for a VAX 11/780. A description of the program, a documented listing, and three examples are presented in this publication. Commentaries and criticisms, particularly from potential or actual users of the program, are welcomed.

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ABSTRACT

A Fortran listing of the quantitative electron microprobe analysis routine, FRAME C, is presented. The source code is extensively documented and there are short summaries of the various parts of the program. Examples are also presented to demonstrate the versatility of the program.

Key words: computer program; electron microprobe; energy-dispersive detector; quantitative analysis; x-ray spectra

I. Introduction

The program FRAME C has been previously described in NBS Technical Note 1106.[1] In that publication, the program was listed in BASIC. This publication contains a listing of the Fortran 77 version of the FRAME C program together with descriptions of the differences between the BASIC and Fortran versions.

The BASIC version was written to run on a specific multi-channel analyzer and had many instructions that were unique to that instrument. The Fortran version was written to operate on a computer that is independent from the multi-channel analyzer. This eliminates all of the analyzer specific instructions from the program and makes the program more universally useful. Anyone operating the program on a computer other than a VAX 11/780* may have to make some alterations to the data file open statements. Also, the subroutine RDFIL was written to read a data file containing an entire spectrum as written by a Tracor Northern* TN 2000 multi-channel analyzer. The user will have to rewrite this subroutine to read the spectral data file as written by his multi-channel analyzer.

The program has been constructed to operate interactively with a minimum of user input. Information from each standard spectrum is processed and stored in a data file. This information is recalled by the program for quantitative analysis computations from the data file. Data files may be stored for future analyses if desired. Since these files are all named, the user may keep as many different files as he desires. The files can be changed at will by the user to include different elements, to change the analytical x-ray lines, or any of the analysis conditions. Some changes require either the same standard spectrum for an element, a new standard spectrum for the element, or merely a change in the list of analyzed elements if the standards are already in the data file.

Some of the equations, particularly those dealing with the relative line intensities, may have been changed in the Fortran version; however, the magnitude of these changes is not very large. As in the BASIC version, the program has been divided into a large number of subroutines. The program listing contains extensive documentation; therefore, we will not describe the individual subroutines.

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* In order to describe adequately materials and experimental procedures, it was necessary to identify commercial products by manufacturer's name or label. In no instance does such identification imply endorsement by the National Bureau of Standards nor does it imply that the particular products or equipment is necessarily the best available for that purpose.

II. Operation Description

A. Input

The input to FRAME C was designed to minimize any operator interactions while at the same time making the program as flexible as possible. The main program determines the path the computation will take as governed by the user's answers to the questions presented by the program. The following section explains the possible answers to the questions in the order that they appear in the program. This is not necessarily the order for any particular analysis. The examples show the questions and answers in the proper order for typical analyses. Note that only the first letter of a Yes or No answer is required, and that the letter must be upper case.

1. Do you wish to create or add to a data file? (Y)es or (N)o

   The program requires a data file for storing all the standards parameters calculated by the program. If this file already exists and no changes are required, answer the question (N)o. If the file does not exist, you must answer (Y)es. An existing file can also be changed by answering (Y)es.

2. Do you wish to add more standard data? (Y)es or (N)o

   After each standard spectrum has been processed, this question is asked. Answer (Y)es if more standard spectra are to be processed or (N)o to begin computing the unknown spectra.

3. Do you wish to change the standard file? (Y)es or (N)o

   After exiting from the computation of unknown spectra, you may alter the standards file by answering (Y)es. This will allow you to run additional standard spectra. If you only wish to change the list of elements analyzed and not the standards themselves, answer (N)o. Also answer (N)o if you have completed your analysis.

4. Do you wish to change the element list? (Y)es or (N)o

   This question follows question 3 if that question is answered (N)o. A (Y)es here will allow you to change the list of elements analyzed in the unknown spectra. A (N)o at this point will terminate the program.

5. Enter name of standard file

   If you are using a previously created standards data file (see question 1) enter the file name of that file. If the standards data file has not been created, enter the file name that you want to create.

6. E0 =

Enter the beam voltage in keV. This is stored in the data file and cannot be changed. All spectra, both standards and unknowns must be run at the same beam voltage.

7. Take-off angle =

Enter the x-ray emergence angle in degrees. This must also be the same for all spectra and cannot be changed once it has been stored in the data file.

8. Number of elements in standard =

Enter the total number of elements in the standard including all unanalyzed elements.

9. Enter Conc., At.No., Line code, & Valence for each

For each element in the standard enter its mass fraction, atomic number, line code (1 = K-line, 2 = L-line, 3 = M-line, 0 = not analyzed), and valence. The valence is used for computing oxygen by stoichiometry - if this calculation is not required, enter zeros for the valence.

10. A file for element ___ already exists - do you wish to replace it?

Enter (Y)es if you wish to change the standard data for the element in question to the current values. Enter (N)o if you wish to retain the old values already stored in the file.

11. Do you wish to change the specimen elements? (Y)es or (N)o

If the unknown computation is entered directly (by answering (N)o to question 1), you can still change the list of elements analyzed, provided that the standards for those elements are present in the data file, by answering (Y)es to this question. (N)o will run the elements as listed in the data file.

12. Number of elements in specimen =

Enter the total number of elements in the unknown specimen including any unanalyzed element. There may only be one unanalyzed element in an unknown.

13. Enter At.No. for each element (unanalyzed last)

Enter the atomic number for each element in the unknown specimen including any unanalyzed element. The preferred order is in order of increasing x-ray peak energy. Any unanalyzed element must, however, be last in the order.

14. Spectrum File name?

    Enter the file name of the data file containing the spectrum (standard or unknown). Typing Control Z terminates processing files and allows the user to alter standard files or to end the program.

15. Enter mean energies for two background points

    The program requires two background regions. The user should enter the two energies that he would like the two regions centered around. The program will then set the regions using the same method as is used for setting peak regions and check to see if any peaks are within the regions. If there are interferences, the next two questions will be asked.

16. Energy ___ interferes with a peak at energy ___
    Do you wish to omit it? (Y)es or (N)o

    If the interference is from a very small peak of a minor element, you may not wish to omit it - enter (N)o. (Y)es will delete that background point.

17. You have too few background points - Try again

    If you omit a background point (question 16), you will not have enough points. The program will ask you for the background points again (question 15) - you will have to enter both background energies again, not just the one you omitted.

In addition, there are many warnings or errors that may be printed if the need should arise. Errors are generated by missing data or problems in opening, reading or writing data files. Warnings usually relate to analytical problems. In some cases, the warnings may help you to select better analytical operating conditions (beam voltage, x-ray line selection, etc.) and in other cases, nothing can be done (x-ray line may be too close to an x-ray absorption edge). In any case, the user should be aware of any conditions that may lead to less than optimum results.

The data file containing the spectrum has a special format on our system. The computer that created the file has only a 16-bit (2 bytes) word instead of the 32-bit (4 bytes) word on the VAX 11/780. Each data point, however, was written into 3 bytes. The data files were written in 512 byte blocks where the first block contains all the header material. If 2048 channels were stored, the next 8 blocks contain the 2048 least significant 2-byte words for each channel and the last 4 blocks contain the 2048 most significant bytes for each channel. The subroutine RDFIL reads this data file and puts the bytes for each data point together into a single number. Unless your spectrum data file has this format, you will have to write a subroutine to read the spectrum data file as formatted at your installation.

B. Output

The output should be reasonably self-explanatory. The standards calculation prints out the multi-element standard factor (MELS), (the computed k-value) for each analyzed element. For a pure element, this value is 1.0. It is printed out for information only; the corrected standard intensity for each element is stored in the standards data file.

The table printed for analysis results contains the atomic number, the mass fraction, the absorption factor (F(X)), and the measured relative intensity ratio (k-value). The total for the analysis is also printed at the end.

C. Examples

In the examples listed below, the > symbol precedes the user input. This symbol does not appear when actually executing the program. The Yes or No answers must be upper case; however, the file name could be either upper or lower case. The symbol ^Z is a Control Z.

Example 1. Create a standard file for two elements, gold and copper, from spectra of each pure element. Then analyze a gold-copper alloy.

```
   Frame C:
  Do you wish to create or add to a data file?
>Y
              *** FRAMEC STANDARDS ***
  Enter name of standard file
>STD
  E0 = >20.
  Take-off angle = >40.
  Number of elements in standard = >1
Enter Conc., At.No., Line code, & Valence for each
>1.,79,2,0
 Spectrum File name? >GOLD20
GOLD STANDARD 20 KEV
Enter mean energies for two background points
>4.3,9.2
MELS = 1.00000
    79      2   28182.67          0
  Do you wish to add more standard data?
>Y
              *** FRAMEC STANDARDS ***
 E0 =  20.0   Take-off angle = 40.0
  Number of elements in standard = >1
Enter Conc., At.No., Line code, & Valence for each
>1.,29,1,0
 Spectrum File name? >COPP20
PURE    COPPER20 KEV
Enter mean energies for two background points
>4.3,9.2
MELS = 1.00000
    29      1   102433.3          0
  Do you wish to add more standard data?
>N
               *** FRAMEC ANALYSIS ***
   Number of elements in specimen =
>2
  Enter At.No. for each element (unanalyzed last)
>79,29
 Spectrum File name? >AU60CU
GOLD 60 COPPER20 KEV
Enter mean energies for two background points
>4.3,9.2
    Z         C         F(X)      K
   79      0.3994    0.9619  0.3296
   29      0.6099    0.9799  0.6579
 TOTAL = 1.0093
               *** FRAMEC ANALYSIS ***
 Spectrum File name? >^Z
  Do you wish to change the standard file? >N
  Do you wish to change the element list? >N
```

Example 2. Analyze a gold-copper alloy using an existing standard file.

```
   Frame C:
  Do you wish to create or add to a data file?
>N
              *** FRAMEC ANALYSIS ***
  Enter name of standard file
>STD
 Do you wish to change the specimen elements?
>N
 Spectrum File name? >GOLD20
GOLD STANDARD 20 KEV
Enter mean energies for two background points
>4.3,9.2
    Z          C          F(X)       K
   79       1.0000     0.9619   1.0000
   29       0.0003     0.9799   0.0004
 TOTAL = 1.0003
              *** FRAMEC ANALYSIS ***
 Spectrum File name? >^Z
  Do you wish to change the standard file?
>N
  Do you wish to change the element list?
>N
```

Example 3. Procedure for optionally changing elemental data in the standard file and then analyzing the gold-copper alloy.

```
   Frame C:
  Do you wish to create or add to a data file?
>Y
              *** FRAMEC STANDARDS ***
  Enter name of standard file
>STD
 E0 =  20.0   Take-off angle = 40.0
  Number of elements in standard = >1
Enter Conc., At.No., Line code, & Valence for each
>1.,79,2,0
 Spectrum File name? >GOLD20
GOLD STANDARD 20 KEV
Enter mean energies for two background points
>4.3,9.2
A file for element  79 already exists - do you wish to replace it? >N
  Do you wish to add more standard data?
>Y
              *** FRAMEC STANDARDS ***
 E0 =  20.0   Take-off angle = 40.0
  Number of elements in standard = >1
Enter Conc., At.No., Line code, & Valence for each
>1.,29,1,0
 Spectrum File name? >COPP20
PURE    COPPER20 KEV
Enter mean energies for two background points
>4.3,9.2
MELS = 1.00000
A file for element  29 already exists - do you wish to replace it? >Y
  Do you wish to add more standard data?
>N
              *** FRAMEC ANALYSIS ***
  Number of elements in specimen =
>1
  Enter At.No. for each element (unanalyzed last)
>79,29
 Spectrum File name? >AU60CU
GOLD 60 COPPER20 KEV
Enter mean energies for two background points
>4.3,9.2
MELS = 1.00000
    Z          C          F(X)       K
   79       0.3994     0.9619   0.3296
   29       0.6099     0.9799   0.6579
 TOTAL = 1.0093
              *** FRAMEC ANALYSIS
 Spectrum File name? >^Z
  Do you wish to change the standard file? >N
  Do you wish to change the element list? >N
```

III. References

1. Myklebust, R.L., Fiori, C.E. and Heinrich, K.F.J., FRAME C: A Compact Procedure for Quantitative Energy-Dispersive Electron Probe X-ray Analysis, NBS Tech. Note 1106, (1979).

IV. Program Listing

```
C        FRAME C MAIN PROGRAM
C
C   Program for quantitative electron probe microanalysis.
C   Written by R.L. Myklebust & B. Thorne
C   National Bureau of Standards
C   Fortran IV+ for a VAX 11/780 vers. VMS 3.0
C
        CHARACTER*10 NAM
        CHARACTER*1 NY,NYE,NYS
    1   FORMAT(A1)
        TYPE *,'   Frame C:'
        TYPE 5
    5   FORMAT('   Do you wish to create or add to a data file? ',$)
        ACCEPT 1,NY
C
C   Add to or create a data file to store the standards information.
C
   10   IOPT=0
        IF(NY.EQ.'Y') THEN
   20      CALL FRCSTD(NAM,IOPT) !standards subroutine
           TYPE 25
   25      FORMAT('   Do you wish to add more standard data? ',$)
           ACCEPT 1,NYE
           IF(NYE.EQ.'Y') GO TO 20
           IOPT=-1
        END IF
   30   CALL FRC(NAM,IOPT)  !specimen subroutine
        IF(IOPT.EQ.1) GO TO 30
        TYPE 35
   35   FORMAT('   Do you wish to change the standard file? ',$)
        ACCEPT 1,NY
        IF(NY.EQ.'Y') GO TO 10
        TYPE 40
   40   FORMAT('   Do you wish to change the element list? ',$)
        ACCEPT 1,NYS
        IF(NYS.EQ.'Y') GO TO 30
        STOP
        END


C        Main FRAMEC program for standards
C
```

```
      SUBROUTINE FRCSTD(NAM,IOPT)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
      INCLUDE 'SPECTM.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'KFAC.CMN'
      INCLUDE 'ROIC.CMN'
C
      INTEGER*2 ZT,LT,QT,NKEY
      CHARACTER*10 NAM
      DIMENSION QM(15)
      TYPE 5
    5 FORMAT('                *** FRAMEC STANDARDS ***')
      IF(IOPT.LT.1) THEN
         TYPE 10
   10    FORMAT('0  Enter name of standard file  ',$)
         READ(5,20) NAM
   20    FORMAT(A10)
      END IF
      IOPT=1
C
C     Open the standards data file if it exists - if it does
C     not exist then create it
C
      OPEN(UNIT=10,FILE=NAM,STATUS='UNKNOWN',ORGANIZATION='INDEXED'
     1 ,FORM='UNFORMATTED',ACCESS='KEYED',KEY=(1:2:INTEGER)
     2 ,RECL=3,RECORDTYPE='VARIABLE',IOSTAT=IOS,ERR=995)
      READ(UNIT=10,KEY=200,KEYID=0,IOSTAT=IOS,ERR=25) ZT,E0,TOA
   25 IF(IOS.EQ.36) THEN  !if new file, ask for input
       TYPE 30
   30  FORMAT('   E0 = ',$)
       ACCEPT *,E0
       TYPE 40
   40  FORMAT('   Take-off angle = ',$)
       ACCEPT *,TOA
       NKEY=200
       WRITE(UNIT=10,IOSTAT=IOS,ERR=990) NKEY,E0,TOA
      ELSE
       IF(IOS.NE.0) GO TO 980
       TYPE 45,E0,TOA   !if old file, print out data
   45 FORMAT('  E0 = ',F5.1,'   Take-off angle = ',F4.1)
      END IF
      CALL COEF(TOA)   !get coefficients
      TYPE 50
   50 FORMAT('   Number of elements in standard = ',$)
      ACCEPT *,N
      TYPE 60
   60 FORMAT(' Enter Conc., At.No., Line code, & Valence for each')
      DO 70 I=1,N
   70 ACCEPT *,XC(I),Z(I),L(I),Q(I)
      Z(N+1)=4   !Be for detector window
      Z(N+2)=14   !Si for detector dead layer
      Z(N+3)=79   !Au for detector
      NX=0
      DO 80 I=N+1,N+3
```

```
   80   L(I)=0
        DO 90 I=1,N+3
        CALL EDGES(I)   !calculate absorption edges
        IF(L(I).GT.0) THEN
         NX=NX+1
         CALL LINES(I)  !calculate x-ray line energies
         LI=L(I)
        IF(Z(I).NE.29) GO TO 81
         IF(EL(LI,I).LT.1.) THEN
          TYPE 85,Z(I)
   85    FORMAT(' The line of ',I3,' is less than 1keV')
          GO TO 999
         END IF
         IF(E(LI*LI,I).GE.E0) THEN
          TYPE 87,Z(I)
   87   FORMAT(' The excitation potential of',I3,' is greater',
     1' than E0')
          GO TO 999
         END IF
        END IF
   90   CONTINUE
        CALL RDSPEC   !get spectrum
        CALL ROI(NX)   !set windows for each element
        N3=1    !set number of iterations to 1
        CALL OCOEF   !calculate overlap factors
        CALL BKG   !calculate background
        CALL OLAPS   !correct for overlaps
        DO 100 I=1,NX
  100   XM(I)=W(I)
        CALL MATRIX(QM,N3)  !do matrix corrections on standards
C
C   Write standards information into data file.
C
        DO 130 I=1,NX
        READ(UNIT=10,KEY=Z(I),KEYID=0,IOSTAT=IOS,ERR=110)ZT,LT,XT,QT
  110   IF(IOS.EQ.36) THEN
         WRITE(UNIT=10,IOSTAT=IOS,ERR=990)Z(I),L(I),XM(I),Q(I)
                TYPE *,Z(I),L(I),XM(I),Q(I)
        ELSE
         TYPE 115,ZT
  115   FORMAT(' A file for element ',I3,' already exists - do you'
     1  ' wish to replace it? ',$)
         ACCEPT 120,NY
  120   FORMAT(A1)
         IF(NY.EQ.'Y') THEN
         REWRITE(UNIT=10,IOSTAT=IOS,ERR=990)Z(I),L(I),XM(I),Q(I)
         END IF
        END IF
  130   CONTINUE
        GO TO 999
  980   TYPE 985,IOS
  985   FORMAT('  Error reading file - error # = ',I5)
        GO TO 999
  990   TYPE 991,IOS
  991   FORMAT('  Error writing file - error # = ',I5)
```

```
      GO TO 999
  995 TYPE 996,IOS
  996 FORMAT('  Error opening file - error # = ',I5)
  999 CLOSE(UNIT=10)
      RETURN
      END


C   Main FRAMEC program for unknown analysis
C
      SUBROUTINE FRC(NAM,IOPT)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'KFAC.CMN'
      INCLUDE 'ROIC.CMN'
      INCLUDE 'SPECTM.CMN'
C
      INTEGER*2 NKEY
      CHARACTER*1 NY
      CHARACTER*10 NAM
      DIMENSION QM(15)
C
    1 FORMAT(A1)
      TYPE 5
    5 FORMAT('               *** FRAMEC ANALYSIS ***')
      IF(IOPT.EQ.0) THEN
         TYPE 10
   10    FORMAT('0   Enter name of standard file  ',$)
         READ(5,20) NAM
   20    FORMAT(A10)
         TYPE 15
   15    FORMAT('0  Do you wish to change the specimen elements'
     1,'? ',$)
         ACCEPT 1,NY
         IF(NY.EQ.'Y') IOPT=-1
      END IF
C
C     Open the standards file - this file is created FRCSTD
C     and contains all information on the standards for the analysis
C
      OPEN(UNIT=10,FILE=NAM,STATUS='OLD',ORGANIZATION='INDEXED',
     1 FORM='UNFORMATTED',ACCESS='KEYED',KEY=(1:2:INTEGER),RECL=3,
     2 RECORDTYPE='VARIABLE',IOSTAT=IOS,ERR=950)
C
C     Read beam voltage and take-off angle - then number of elements
C
      READ(UNIT=10,KEY=200,KEYID=0,IOSTAT=IOS,ERR=990) NKEY,E0,TOA
      READ(UNIT=10,KEY=201,KEYID=0,IOSTAT=IOS,ERR=25) NKEY,N
   25 IF((IOS.EQ.0).AND.(IOPT.EQ.-1)) THEN
       GO TO 27
      ELSE IF(IOS.EQ.36) THEN
   27  TYPE 30  !create or change element table
   30 FORMAT('   Number of elements in specimen = ',$)
```

```
        ACCEPT *,N
        TYPE 40
 40     FORMAT('   Enter At.No. for each element (unanalyzed last)')
        ACCEPT *,(Z(I),I=1,N)
 50        IF(IOPT.EQ.-1) THEN !rewrite the table
        REWRITE(UNIT=10,IOSTAT=IOS,ERR=980) NKEY,N
        READ(UNIT=10,IOSTAT=IOS,ERR=940) NKEY
        REWRITE(UNIT=10,IOSTAT=IOS,ERR=980) NKEY,(Z(I),I=1,N)
           ELSE  !create the element table
        NKEY=201
        WRITE(UNIT=10,IOSTAT=IOS,ERR=980) NKEY,N
        NKEY=202
        WRITE(UNIT=10,IOSTAT=IOS,ERR=980) NKEY,(Z(I),I=1,N)
           END IF
        ELSE
        IF(IOS.NE.0) GO TO 970
        READ(UNIT=10,KEY=202,KEYID=0,IOSTAT=IOS,ERR=990)
     1  NKEY,(Z(I),I=1,N)
        END IF
        IOPT=1
C
C   Read in the standards data for each element
C
        NX=N
        DO 100 I=1,N
        READ(UNIT=10,KEY=Z(I),KEYID=0,IOSTAT=IOS,ERR=60)NKEY,L(I),
     1  QM(I),Q(I)
C
C   See if the element is present in the file
C
 60     IF(IOS.EQ.36) THEN
         IF(I.EQ.N) THEN
          NX=N-1
          L(I)=0
         ELSE
          TYPE 65,Z(I)
 65      FORMAT('   Standard file missing for element ',I3)
          GO TO 999
         END IF
        ELSE
         IF(IOS.NE.0) GO TO 960
        END IF
100     CONTINUE
        Z(N+1)=4  !Be for detector window
        Z(N+2)=14  !Si for detector window
        Z(N+3)=79  !Au for detector window
        DO 110 I=N+1,N+3
110     L(I)=0
        CALL COEF(TOA)  !get coefficients
        DO 120 I=1,N+3
        CALL EDGES(I)  !calculate absorption edges
        IF(L(I).GT.0) THEN
         CALL LINES(I) !calculate x-ray line energies
        END IF
120     CONTINUE
```

```
        CALL RDSPEC(IOPT) !get the spectrum
        IF(IOPT.EQ.-1) GO TO 999
        CALL ROI(NX)  !set peak windows for each element
        N3=3
        CALL OCOEF  !calculate overlap coefficients
        CALL MATRIX(QM,N3) !do matrix corrections ZAF
        GO TO 999
C
C   Error conditions for reading, writing and opening files
C
  940   TYPE 945,IOS
  945   FORMAT('  Error reading element list - error # = ',I5)
        GO TO 999
  950   TYPE 955,IOS
  955   FORMAT('  Error opening data file - error # = ',I5)
        GO TO 999
  960   TYPE 965,IOS
  965   FORMAT('  Error reading element entry - error # = ',I5)
        GO TO 999
  970   TYPE 975,IOS
  975   FORMAT('  Error reading number of elements - error # = ',I5)
        GO TO 999
  980   IF(IOS.EQ.53) THEN !if record does not exist, change
         IOPT=1  !to write a new record.
         GO TO 50 !try again
        ELSE
         TYPE 985,IOS
  985   FORMAT('  Error writing no. of elements or element list -'
     1  ,' error # = ',I5)
        END IF
        GO TO 999
  990   TYPE 995,IOS
  995   FORMAT('  Error reading E0 & TOA - error # = ',I5)
  999   CLOSE(UNIT=10)
        RETURN
        END



      SUBROUTINE ABSFAC(E1,F1,T2)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'GEOM.CMN'
C
C  Absorption factor - E1 is the excitation potential
C
      X3=T2*Q1   !absorption coef * csc(take-off angle)
      GA=(E0**1.65-E1**1.65)*Q2 !gamma in Heinrich's eqn.
      F1=1/(1+1.2E-6*GA*X3)**2 !f(chi)
      RETURN
      END



      SUBROUTINE AREA(I,E7,E1,O1,E8,E9)
C
```

```
C       Compute the area of the Gaussian peak that is integrated
C       within the energy window for each element.
C
      INCLUDE 'ROIC.CMN'
      E3=EHI(I)    !upper energy of window
      E2=ELOW(I)   !lower energy of window
      X2=(E2-E7)/S1(E1)/1.4142 !factor required by integration routine
      CALL GAUS(E8,E9,X2) !integrate low energy side
      CALL ICHG(E7,G4)  !add in incomplete charge effect
      TE=ABS(E8)/2  !integral from low to peak energy
      X2=(E3-E7)/S1(E1)/1.4142 !factor required by integration routine
      CALL GAUS(E8,E9,X2) !integrate high energy side
      E8=ABS(E8)/2  !integral from peak to high energy
      IF(E2.LT.E7)GO TO 100
      O1=E8-TE   !window on high side of peak
      RETURN
  100 IF(E3.GT.E7)GO TO 200
      O1=TE-E8+G4  !window on low side of peak
      RETURN
  200 O1=TE+E8+G4  !peak energy inside window
      RETURN
      END



C   This is the FRAME C background calculation
C
        SUBROUTINE BKG
        INCLUDE 'ABSB.CMN'
        INCLUDE 'BLNK.CMN'
        INCLUDE 'CONC.CMN'
        INCLUDE 'ENER.CMN'
        INCLUDE 'KFAC.CMN'
        INCLUDE 'ROIC.CMN'
C
        DIMENSION X(2),Y(2),U(2)
        DO 40 I=1,NB
        E2=ELOW(I)  !low energy of bg window
        E3=EHI(I)  !high energy of bg window
        T5=CNTS(I)  !counts in bg window
        X1=T5/(E3-E2+.01)/100. !counts per channel in bg window
        E1=(E2+E3)/2.  !centroid energy of bg window
        T2=0.
           DO 10 J=1,N
           CALL MAC(E1,FA,J)
           T2=T2+XC(J)*FA !concentration average of abs. coef.
   10      CONTINUE
        CALL DET(ED,E1,N) !detector efficiency ED
        CALL ABSFAC(E1,F1,T2) !f(chi) F1
        T1=ED*F1/E1
        X(I)=E0-E1
        Y(I)=X1/T1
        U(I)=X(I)**2
   40   CONTINUE
C
```

```
C       Set up matrix for fit to background
C
        D1=X(1)*U(2)-U(1)*X(2)
        XK1=(Y(2)*X(1)-Y(1)*X(2))/D1
        XK2=(Y(1)*U(2)-Y(2)*U(1))/D1
        IF(L(1).EQ.20) GO TO 999 !exit if determining detector param.
        DO 60 I=1,N
        IF(L(I).EQ.0) GO TO 60 !skip if unanalyzed element
        L1=L(I)
        E1=EL(L1,I)  !energy of peak
        T5=CNTS(I+NB)  !counts in peak window
        T2=0.
           DO 50 J=1,N
           CALL MAC(E1,FA,J)
           T2=T2+XC(J)*FA !concentration average of peak abs. coef.
   50      CONTINUE
        CALL DET(ED,E1,N) !detector efficiency for peak energy
        LEG=L1*L1
        E4=E(LEG,I)  !excitation potential for peak
        CALL ABSFAC(E4,F1,T2) !f(chi) for peak
        T1=ED*F1/E1
        X1=E0-E1
        G1=T1*(XK1*X1*X1+XK2*X1) !bg per channel at peak energy
        GS=100.*(EHI(I+NB)-ELOW(I+NB)+.01) !number of channels in
                                                !window
        XM(I)=T5-G1*GS  !bg corrected peak intensity
C       TYPE *,'BKG ',T5,G1,GS,ED,F1
   60   CONTINUE
  999   RETURN
        END



      SUBROUTINE COEF(TOA)
      INCLUDE 'KBKA.CMN'
      INCLUDE 'ATWT.CMN'
      INCLUDE 'GEOM.CMN'
      INCLUDE 'DETECT.CMN'
C
C  Coef. for calculations
C
C       Kb/Ka ratios
C
      DATA VB/10*0.,.011,.027,.04,.055,.066,.078,.085,.097,.108
     2,.114,.115,.117,.119,.119,.121,.121,.121,.123,.1235,.125/
C
C       Table of atomic weights
C
      DATA WA/1.,4.,6.94,9.013,10.82,12.011,14.007,16.,19.,20.18,22.99
     2,24.31,26.98,28.09,30.97,32.06,35.45,39.95,39.1,40.08,44.96,47.9
     3,50.94,52.,54.94,55.85,58.93,58.71,63.54,65.37,69.72,72.59,74.92
     4,78.96,79.91,83.8,85.47,87.62,88.91,91.22,92.91,95.94,99.,101.1
     5,102.9,106.4,107.9,112.4,114.8,118.7,121.8,127.6,126.9,131.3
     6,132.9,137.3,138.9,140.1,140.9,144.2,145.,150.4,152.,157.,158.9
     7,162.5,164.9,167.3,168.9,173.,175.,178.5,180.95,183.85,186.2
```

```
     8,190.2,192.2,195.1,196.97,200.6,204.4,207.2,209.,210.,210.,222.
     9,223.,226.,227.,232.,231.,238.,237.,244.,243.,247.,247.,251.
     0,254./
      Q3=149.   !resolution of Si detector (eV on MnKa)
      Q2=90.   !beam incidence angle
      P6=1.57E-3  !thickness of Be window (fitted from C)
      P7=9.76E-6  !thickness of Si dead layer (fitted)
      Q3=Q3**2-14737.5  !noise factor for peak width calc.
      Q1=1/SIN(TOA/57.2958) !csc(take-off angle)
      Q2= SIN(Q2/57.2958) !sine of beam incidence angle
      RETURN
      END



      SUBROUTINE CONAVE(I,S2,T2,X2)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
      INCLUDE 'ZAFF.CMN'
C
C   Concentration ave. factors
C
      S2=0.
      X2=0.
      T2=0.
      DO 100 J=1,N
      S2=S2+XC(J)*S(J,I) !conc. ave. of stopping power
      X2=X2+XC(J)*V(J,I) !conc. ave. of R factor
      T2=T2+XC(J)*H(J,I) !conc. ave. of absorption coef.
  100 CONTINUE
  999 RETURN
      END



      SUBROUTINE DET(ED,E1,N)
      INCLUDE 'DETECT.CMN'
C
C  Detector efficiency
C
      I=N+1
      CALL MAC(E1,FA,I)  !abs. coef. for Be
      T3=FA*1.82*P6  !linear absorption in Be window
      I=N+3
      CALL MAC(E1,FA,I)  !abs. coef. for Au
      T4=FA*19.3*8.E-7  !linear absorption in Au layer
      I=N+2
      CALL MAC(E1,FA,I)  !abs. coef. for Si
C
C       Detector efficiency - the last term is for high energy X-rays
C       that may be lost by passing through the detector without being
C       absorbed. (detector is 0.3 cm thick)
C
      ED=EXP(-T3-T4-FA*2.33*P7)*(1-EXP(-FA*2.33*.3))
      RETURN
```

```
      END


      SUBROUTINE DIST(S3)
      INCLUDE 'ATWT.CMN'
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
      INCLUDE 'ENER.CMN'
C
C  Compute element by difference or stoichiometry
C
      S3=0.
      DO 20 I=1,N
      IF(L(I).EQ.0)GO TO 20 !do not sum unanalyzed element
      IF(XC(I).GT.0.)GO TO 10 !do not sum any negative conc.
      XC(I)=0.
   10 S3=S3+XC(I)  !S3 is the sum of the calculated conc.
   20 CONTINUE
      IF(L(N).GT.0)GO TO 999 !skip if all elements analyzed
      IF(Q(1).GT.0.)GO TO 30 !skip if stoichiometry calc.
      XC(N)=1-S3  !calc. last element by difference
      S3=1
      GO TO 999
C
C       Stoichiometry calculation
C
   30 XC(N)=0
      DO 50 I=1,N-1
      F3=.5*XC(I)*Q(I)*WA(Z(N))/WA(Z(I))  !calc. oxygen by stoic.
      XC(N)=XC(N)+F3  !sum all oxygen concentrations
   50 CONTINUE
      S3=S3+XC(N)  !add oxygen conc. to sum of elements
  999 RETURN
      END


      SUBROUTINE EDGES(I)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'ENER.CMN'
C
C  Absorption edges
C       All edges are computed for each element whether they exist or
C       not. This fit is NOT good below 1keV.
C
      DIMENSION TD(4),XE(3,9)
      DATA XE/-.0397931,2.423,-5.5091,-.033916,2.82526,-9.03526,
     2-.0865397,3.32315,-10.2505,-.228343,4.31172,-12.0025,1.25179,
     3-7.838,11.5803,.834903,-4.14925,3.33802,.442217,-.979241,
     4-3.15348,.25141,.931913,-8.03561,.272951,.688906,-7.4243/
      ZR=Z(I)   !atomic number (int->real)
      Z1=LOG(ZR)
      DO 100 M1=1,9  !calc. all edges for element Z(I)
      E(M1,I)=EXP(Z1*Z1*XE(1,M1)+XE(2,M1)*Z1+XE(3,M1))
```

```
      IF(M1.EQ.1)GO TO 100
      IF(E(1,I).GT.4)GO TO 100 !skip very low energy L and M lines -
      E(M1,I)=0.  !K-edge is less than 4keV
  100 CONTINUE
      RETURN
      END



      SUBROUTINE ESP(I,N,E6,E7,S7,S8,YD)
C
C       Calculate counts in escape peak
C
      O1=0.
      IF(E7.LT.1.838)GO TO 999     !skip if peak E<Si energy
      E1=E7
      E7=E7-1.74      !energy of escape peak
      IF(E6.LT.E7-YD.OR.E6.GT.E7+YD) THEN  !see if escape peak
                                           !interfers
        II=N+2
        CALL MAC(E1,FA,II)     !abs. coef. of line in Si
        S7=.5*(1-327.9/FA*LOG(1+FA/327.9))
        S8=.038*S7/(1-.038*S7)     !relative weight of escape peak
        E7=S1(E7)      !sigma (width) of escape peak
        CALL AREA(I,E7,E1,O1,E8,E9)    !integral of overlap portion
      END IF
  999 RETURN
      END



      SUBROUTINE FACTOR(E1,F1,F2,I,S2,T2,X2,W1)
      INCLUDE 'ABSB.CMN'
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
      INCLUDE 'FLUOR.CMN'
      INCLUDE 'GEOM.CMN'
      INCLUDE 'ZAFF.CMN'
C
C  Correction factors in loop
C
      W1=(V(I,I)*S2)/(S(I,I)*X2) !atomic number factor
      F(2,I)=F1    !f(chi) for specimen
      F2=0
      DO 200 J=1,N
      IF(AP(I,J).EQ.0)GO TO 200  !skip if no fluorescence correction
      T3=0.
      DO 100 I1=1,N
      T3=T3+XC(I1)*H(I1+15,J)  !abs. coef. of exciting line in spec.
  100 CONTINUE
      X1=Q1*T2/T3
      GB=333000./((E0**1.65)-(E1**1.65))/T3*Q2
      F4=LOG(1+X1)/X1+LOG(1+GB)/GB
      F2=F2+XC(J)*O(I,J)/T3*F4  !sum of fluor. of element I
  200 CONTINUE
```

```
  999 RETURN
      END



      FUNCTION FT2(E1)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
C
C   Conc average of absorp. coef. for overlap correction
C
      FT2=0.
      DO 100 I=1,N
      CALL MAC(E1,FA,I)  !calculate absorption coef. for energy E1
      FT2=FT2+XC(I)*FA  !conc. average of absorption coef.
  100 CONTINUE
      RETURN
      END



      SUBROUTINE GAUS(E8,E9,X2)
C
C  Integrate Gaussian -
C         this routine, when it is called with the proper
C         arguments, will integrate a Gaussian between two
C         points symetrically placed with respect to the
C         centroid of the Gaussian.
C
C
      S27=-27
      T1=2.**S27
      IF(X2.EQ.0)GO TO 900
      Y1=ABS(X2)
      Y2=Y1*Y1
      IF(Y1.LE.1)GO TO 100
      YC=2.**3.5
      U1=.83*YC
      S6=2.**(YC*YC-8)
      IF(Y1.LE.U1)GO TO 400
      E8=1.
      E9=0.
      GO TO 300
  100 W2=0.
      A1=1.
      T2=1.
      P2=2*Y2
  200 A1=A1+2
      T2=P2*T2/A1
      S2=T2+S2
      IF(T2.GE.T1)GO TO 200
      E8=(S2+1)*1.12838*Y1*EXP(-Y2)
      E9=1-E8
  300 IF(X2.GE.0)GO TO 999
      E9=2-E9
```

```
  400 F2=0
      GS=1
      F1=2*X1
      GI=2*Y2+1
      P3=F1/GI
      A2=1.
      YB=GI+4
  500 F5=-A2*(A2+1)
      F3=YB*F1+F5*F2
      G3=YB*GI+F5*GS
      F4=F3/G3
      IF(ABS(1-F4/P3).GT.T1)GO TO 800
      IF(P3.GT.F4)GO TO 700
      IF(G3.LT.56)GO TO 600
      F3=F3/S6
      G3=G3/S6
      F1=F1/S6
      GI=GI/S6
  600 F2=F1
      GS=GI
      F1=F3
      GI=G3
      A2=A2+2
      YB=YB+4
      P3=F4
      GO TO 500
  700 F4=P3
  800 E9=F4*EXP(-Y2)*1.12838/2
      E8=1-E9
      GO TO 300
  900 E8=0.
      E9=1.
  999 RETURN
      END



      SUBROUTINE ICHG(E7,G4,J)
C
C       Compute incomplete charge correction
C
      INCLUDE 'ROIC.CMN'
      E2=ELOW(J+NB)    !low energy side of window
      E3=EHI(J+NB)    !high energy side of window
      G4=0.
        X1=6.
        X3=.1
        IF(E7.GE.6.4)GO TO 10  !select the constants for the fit
        X1=.86*E7*E7-7.44*E7+18.34
        X3=-.0168*E7*E7+.141*E7-.115
        IF(X3.LE.0)GO TO 999  !if X3 too small, exit
   10   IF(E2.GE.E7)GO TO 999  !exit if E2 on high energy side
        X2=(E2-E7)/X3
        G4=X1*X3*X3*(1-EXP(X2)*(1-X2)) !result for low energy side of
                                       !window
```

```
      IF(E3.GE.E7)GO TO 999  !exit if E3 on high energy side
      X2=(E3-E7)/X3
      G4=G4-X1*X3*X3*(1-EXP(X2)*(1-X2)) !result for high energy side
999   RETURN
      END


      SUBROUTINE LINES(I)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'ENER.CMN'
C
C  Line energies
C       All lines are computed for each element whether they exist or
C       not. This fit is NOT good for lines below 1keV.
C
      DIMENSION T(3,17)
      DATA T/-.0199726,2.22412,-5.1774,-.123941,3.29533,
     2-9.75836,-.47555,6.84662,-20.0833,-.060101,2.52781,-5.6437,
     3-.117102,3.22414,-9.58711,-.192466,3.83158,-10.9293,-.197431,
     44.01718,-11.3323,-.00322523,2.48613,-8.37742,.035676,2.29113,
     5-8.09392,.00288553,2.49221,-8.60965,.0957107,1.69157,-6.76302
     6,.092961,1.7559,-6.81839,.0505888,2.0035,-7.30182,-.390705,
     76.17432,-19.0119,-.386042,6.14822,-18.7034,-.603132,7.75598
     8,-21.4878,.322877,.102358,-5.58269/
      RZ=Z(I)
      Z1=LOG(RZ)  !log of atomic number of element
      DO 100 M1=1,17  !calculate all x-ray lines for element
      EL(M1,I)=EXP(Z1*Z1*T(1,M1)+T(2,M1)*Z1+T(3,M1))
100   CONTINUE
      RETURN
      END


      SUBROUTINE MAC(E1,FA,I)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'ENER.CMN'
C
C  Mass absorption coef.
C       E1 is the energy of the x-ray line being absorbed. FA is the
C       absorption coefficient and I is the index of the absorber.
C
      DIMENSION GJ(3),GK(3),R(10),XD(4,4)
C       R is edge jump ratio
      DATA R/1.,1.,1.17,1.63,1.,1.16,1.4,1.621,1.783,1./
      DATA GJ/-.0045522,-.0068535,1.070181/
      DATA GK/-.1131595,.8368829,-.5459687/
      DATA XD/-.2322294,4.070053,-6.220746,1.,-.2544711
     2,4.769245,-10.37878,2.73,.2562163
     3,1.15119,-5.684848,2.6,1.359165,-9.492116
     4,18.64081,2.22/
        XD(4,2)=2.73
      RZ=Z(I)      !absorber atomic number
      Z1=LOG(RZ)     !log of atomic number
```

```
      XD(4,1)=EXP(GJ(1)*Z1*Z1+GJ(2)*Z1+GJ(3))
      IF(Z(I).LT.42)GO TO 100   !select XD constant
      XD(4,2)=EXP(GK(1)*Z1*Z1+GK(2)*Z1+GK(3))
  100 DO 300 M1=1,10
      IF(M1.EQ.10)GO TO 200   !scan edges
      IF(E1.LT.E(M1,I))GO TO 300
  200 L1=M1-INT(M1/3)-INT(M1/4)-INT(M1/7) !select proper edge
C
C       M1      L1      edge
C       1       1       K
C       2       2       L1
C       3       2       L2
C       4       2       L3
C       5       3       M1
C       6       3       M2
C       7       3       M3
C       8       3       M4
C       9       3       M5
C       10      4       N1
C
      ZC=EXP(XD(1,L1)*Z1*Z1+XD(2,L1)*Z1+XD(3,L1))/R(M1)
      FA=ZC*(12.398/E1)**XD(4,L1)  !absorption coefficient
        RETURN
  300 CONTINUE
      RETURN
      END



      SUBROUTINE MATRIX(QM,N3)
      INCLUDE 'ABSB.CMN'
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'FLUOR.CMN'
      INCLUDE 'KFAC.CMN'
      INCLUDE 'ROIC.CMN'
      INCLUDE 'ZAFF.CMN'
C
C   Matrix corrections
C
      DIMENSION QM(15),U(15),UB(15),UC(15)
      DIMENSION VZ(15,15)
      N1=0
      DO 200 J=1,15
      DO 100 I=1,15
      AP(I,J)=0.  !initialize fluorescence matrix
  100 CONTINUE
  200 CONTINUE
      DO 300 J=1,N
      IF(L(J).EQ.0)GO TO 300
      CALL SETUP(J)  !set up conc. independent parameters
  300 CONTINUE
      IF(N3.EQ.1)GO TO 500 !skip if calculating a standard
      S3=0
```

```
      DO 400 I=1,N
      IF(L(I).EQ.0)GO TO 450
      JJ=NB+I   !JJ is the region number for peak I
      T5=CNTS(JJ)  !integrated counts in region JJ
      XM(I)=T5/QM(I)  !relative intensity (k-value)
      UB(I)=XM(I)
      XC(I)=XM(I)  !assume conc. equal to k-value
        IF(XC(I).GT.1.) XC(I)=1.
      AZ=0.
  400 CONTINUE
  450 CALL DIST(S3)  !calc. method for unanalyzed element
      CALL NORM(S3)  !normalize concentrations
      AZ=1.
  500 DO 900 I=1,N3  !begin iteration loop
 1100 DO 1200 IJ=1,N
      IF(L(IJ).EQ.0)GO TO 1180 !skip if element unanalyzed
      CALL CONAVE(IJ,S2,T2,X2) !conc. average of S, R, and absorp.
                               !coef.
      L1=L(IJ)
      E1=EL(L1,IJ)  !line energy
      E2=E(L1*L1,IJ)  !edge energy
      CALL ABSFAC(E2,F1,T2) !get absorption coefficients
      CALL FACTOR(E2,F1,F2,IJ,S2,T2,X2,W1) !get matrix factors
      IF(XC(IJ).EQ.0)GO TO 1200
      G3=XC(IJ)/W1*(1+F2)*F(2,IJ)/F(1,IJ) !k-value for conc. XC
C       WRITE(6,*) W1,F2,F(2,IJ)/F(1,IJ)
      IF(N3.GT.1)GO TO 1180 !skip if calculating an unknown
      XM(IJ)=XM(IJ)/G3  !counts for pure element (store in file)
      WRITE(6,1160)G3
 1160 FORMAT(' MELS =',F8.5)
      GO TO 1200  !skip if calculating a standard
 1180 IF(XM(IJ).EQ.1.OR.XC(IJ).EQ.1)GO TO 1200
      G4=XM(IJ)*XC(IJ)    !new concentration by
      UB(IJ)=G4*(1-G3)/(G4+G3*(1-XM(IJ)-XC(IJ)))!hyperbolic equation
 1200 CONTINUE
        DO 1210 IJ=1,N
 1210   XC(IJ)=UB(IJ)  !replace old conc. with new conc.
      CALL DIST(S3)  !calc. method for unanalyzed element
      IF(N3.EQ.1)GO TO 9999 !skip to end if calculating a standard
      IF(I.EQ.N3)GO TO 910 !skip if iteration complete
      CALL NORM(S3)  !normalize concentrations
      CALL BKG   !do background correction
      CALL OLAPS  !do overlap corrections
      DO 800 IJ=1,N
      IF(L(IJ).EQ.0)GO TO 580
      XM(IJ)=W(IJ)/QM(IJ) !recalculate k-values
  580 U(IJ)=0.
  800 CONTINUE
  900 CONTINUE   !end of iteration loop
  910 WRITE(6,920)  !write headings for output
  920 FORMAT(5X,'Z',9X,'C',9X,'F(X)',6X,'K')
  940 FORMAT(' ',2X,I3,6X,F6.4)
  960 FORMAT(' ',2X,I3,6X,F6.4,4X,F6.4,2X,F6.4)
      DO 1000 I=1,N
      IF(L(I).EQ.0)WRITE(6,940)Z(I),XC(I)  !unanalyzed element
```

```
      IF(L(I).GT.0)WRITE(6,960)Z(I),XC(I),F(1,I),XM(I) !analyzed
                                                       !element
 1000 CONTINUE
      WRITE(6,1020)S3  !output analysis total
 1020 FORMAT(1H0,' TOTAL = ',F6.4)
 9999 RETURN
      END



      SUBROUTINE NORM(S3)
      INCLUDE 'BLNK.CMN'
      INCLUDE 'CONC.CMN'
C
C       Normalize concentrations to 100%
C
      DO 100 I=1,N
      XC(I)=XC(I)/S3  !S3 is sum of concentrations
  100 CONTINUE
      RETURN
      END



      SUBROUTINE OCOEF
      INCLUDE 'ABSB.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'GEOM.CMN'
      INCLUDE 'ROIC.CMN'
      INCLUDE 'ZAFF.CMN'
C
        DIMENSION WQ(15)
C
C    Compute overlap coefficients
C
      DO 500 J=1,N
      IF(L(J).EQ.0)GO TO 500  !skip if element not analyzed
      L1=L(J)
      E7=EL(L1,J)   !energy of x-ray line
      E2=ELOW(J+NB)    !low energy of window (E2)
      E3=EHI(J+NB)     !high energy of window (E3)
      X2=(E2-E7)/S1(E7)/1.4142  !Gaussian integration factor (low)
      CALL GAUS(E8,E9,X2)  !integrate Gaussian peak
      CALL ICHG(E7,G4,J)  !calc. incomplete charge collection
      E5=ABS(E8)/2   !integral - centroid to low energy
      X2=(E3-E7)/S1(E7)/1.4142  !Gaussian integration factor (high)
      CALL GAUS(E8,E9,X2)  !integrate Gaussian peak
      E4=ABS(E8)/2   !integral - centroid to high energy
      IF(E2.LE.E7)GO TO 100
      WQ(J)=E4-E5   !E2>peak energy
      GO TO 300
  100 IF(E3.GE.E7)GO TO 200
      WQ(J)=E5-E4+G4   !E3<peak energy
      GO TO 300
  200 WQ(J)=E5+E4+G4   !E2<peak energy>E3
```

```
  300 CONTINUE
  500 CONTINUE
        DO 650 J=1,12
        DO 600 I1=1,12
        DO 550 IJ=1,17
  550   HI(IJ,J,I1)=0.   !initialize overlap factors
  600   CONTINUE
  650   CONTINUE
      DO 900 K1=1,2   !1=self overlap, 2=other overlap
      DO 800 I1=1,N   !I1=analyzed line to be checked
      IF(L(I1).EQ.0)GO TO 800  !skip if unanalyzed element
      L1=L(I1)
      E6=EL(L1,I1)   !line energy of analyzed line
      YD=4*S1(E6)   !4*sigma of analyzed line
        E2=ELOW(I1+NB)   !low energy of window for I1
        E3=EHI(I1+NB)   !high energy of window for I1
      DO 700 J=1,N   !J=possible overlapping line
        L2=L(J)    !line code for measured line of J
      IF(L2.EQ.0)GO TO 700  !skip if not an analyzed line
C
C       Next two lines have the following effect:
C       If K1=2, skip if I1 and J are the same element.
C       If K1=1, skip if I1 and J are NOT the same element.
C
      IF((K1.EQ.2).AND.(I1.EQ.J))GO TO 700
      IF((I1.NE.J).AND.(K1.EQ.1))GO TO 700
      IF(L2.EQ.1)GO TO 680  !L2 is a K line
      X2=1/LOG(E0*E0/E(4,J)/E(9,J)) !define X2 for L and M lines
      GO TO 690
  680 X2=1    !define X2 for K lines
  690 CALL OLAP(WQ,E6,J,I1)  !calc. overlap coefficient
  700 CONTINUE
  800 CONTINUE
  900 CONTINUE
      RETURN
      END



      SUBROUTINE OLAP(WQ,E6,J,I1)
      INCLUDE 'ABSB.CMN'
      INCLUDE 'BLNK.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'KBKA.CMN'
      INCLUDE 'GEOM.CMN'
C
C  Overlap for each line
C
      DIMENSION U(15),X(15),WQ(15),S(17,15)
      CALL YIELD(J,X(1),X(2),X(3))  !get fluorescence yield
      DO 100 L2=1,9    !scan each absorp. edge
      IF(E(L2,J).EQ.0)GO TO 9999  !skip if edge energy=0
      I2=L2-INT(L2/3)-INT(L2/4)-INT(L2/7) !edge number
      M3=2*(INT(L2/I2)-INT(L2/6)+INT(L2/7)) !electrons per shell
C
```

```
C       L2      I2      M3
C       1       1       2
C       2       2       2
C       3       2       2
C       4       2       4
C       5       3       2
C       6       3       2
C       7       3       4
C       8       3       4
C       9       3       6
C
      IF(E(L2,J).GE.E0)GO TO 100  !skip if edge energy>E0
      E1=E0/E(L2,J)    !overvoltage
      E4=1166*E(L2,J)/XJ(Z(J))
      X1=E1*E4
C       Compute the cross-section function
      U(L2)=M3*(E1-1-LOG(E4)/E4*2.905*(SQRT(X1)-SQRT(E4)))*X(I2)
  100 CONTINUE
      V5=1.
      V4=1.
      V3=1.
      V2=1.
      V1=1.
C
C   Calculate line weights ZF & ZM  (these are empirical fits)
C
      ZF=.2567*Z(J)-6.8176
      ZM=EXP(34.165*X2-30.027*SQRT(X2)+8.5268)/1.6
C
C       Set up cross-section ratios for K-L and L-M lines
C
      GO TO (120,200,300),L(J)   !sort K,L, or M lines
  120 V2=U(4)/U(1)*ZF  !K to L3 edge
      V4=U(2)/U(1)*ZF  !K to L1 edge
      V5=U(3)/U(1)*ZF  !K to L2 edge
      GO TO 400
  200 V1=U(1)/U(4)/ZF  !L3 to K edge
      V3=ZM   !L3 to M edges
      V4=U(2)/U(4)  !L3 to L1 edge
      V5=U(3)/U(4)  !L3 to L2 edge
      GO TO 400
  300 V2=1/ZM   !M to L3 edge
      V4=U(2)/U(4)/ZM  !M to L1 edge
      V5=U(3)/U(4)/ZM  !M to L2 edge
C
C       The S values that follow are line intensities relative to the
C       measured line for each element. For example, S(1,J) is the
C       relative intensity for the Ka line. If the Ka line is
C       measured, then S(1,J)=1. If the La line is measured, then
C       S(1,J)= the V1 computed above in line 200.
C
  400 S(1,J)=V1    !Ka
      IF(Z(J).GT.30)GO TO 500 !select the Kb/Ka ratio
      R1=VB(Z(J))
      IF(Z(J).LE.30.)GO TO 600
```

```
  500 RZ=Z(J)
      R1=.115*LOG(RZ)-2.3 !compute Kb/Ka for elements>(Z=30)
  600 S(2,J)=V2     !La1
      S(3,J)=V3     !Ma
      S(4,J)=R1/(1-R1)*V1  !Kb
      S(5,J)=.1*V2    !La2
      S(6,J)=.044*V2    !L1
      S(7,J)=V2*(.2808-.0016*Z(J)) !Lb2
      S(8,J)=V5     !Lb1
      S(9,J)=.154*V5    !Lg1
      S(10,J)=.02*V5    !Ln
      S(11,J)=.166*V4    !Lb3
      S(12,J)=.068*V4    !Lg3
      S(13,J)=.104*V4    !Lb4
      S(14,J)=.06*V3    !Mz1
      S(15,J)=.5*V3*U(9)/U(10)  !Mb
      S(16,J)=.05*V3*U(8)/U(10)  !Mg
      S(17,J)=.01*V3*U(7)/U(10)  !M2N4
      IF(I1.EQ.J)GO TO 820  !skip if for self-overlap
      DO 800 I2=1,17
      IF(S(I2,J).GT.0)GO TO 800 !make sure all overlaps are positive
      S(I2,J)=0.  !or zero
  800 CONTINUE
C
C       Test for overlaps and compute the relative overlapping area
C
  820 DO 1100 I2=1,17
      S8=1
      E7=EL(I2,J)  !line energy
      IF(E6.EQ.E7.OR.E7.LT.1..OR.E7.GT.E0.OR.E7.LT.E6-YD)GO TO 1100
      SIG=S1(E7)  !peak width (sigma)
      IF(E7.LT.E6+YD)GO TO 900
      CALL ESP(J,N,E6,E7,S7,S8,YD) !check for escape peak overlap
  900 CALL AREA(J,E7,E1,O1,E8,E9) !get overlapping area
      IF(K1.EQ.2)GO TO 1000
      IF(I2.EQ.L(J)) GO TO 1100
      WQ(J)=WQ(J)+O1*S(I2,J)  !sum of self-overlaps
        GO TO 1100
 1000 HI(I2,J,I1)=O1/WQ(J)*S8*S(I2,J) !store each overlap
 1100 CONTINUE
 9999 RETURN
      END



      SUBROUTINE OLAPS
      INCLUDE 'ABSB.CMN'
      INCLUDE 'BLNK.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'KFAC.CMN'
      INCLUDE 'LINEDG.CMN'
C
C  Correct overlaps for each line
C
      DO 100 J=1,N  !get parameters for each element
```

```
      IF(L(J).EQ.0)GO TO 100 !skip if not analyzed
      L1=L(J)
      E1=EL(L1,J)  !line energy
      L6=LED(L1)
      E2=E(L6,J)  !edge energy
      CALL DET(ED,E1,N)  !detector efficiency (det. eff.)
        T2=FT2(E1)  !conc. average of absorption coef.
      CALL ABSFAC(E2,F1,T2) !absorption factor f(chi)
      F(4,J)=F1*ED  !store f(chi)*(det. eff.)
      W(J)=XM(J)  !both W and XM contain measured intensity
  100 CONTINUE
      DO 400 JA=1,3  !iterate the overlap correction
      DO 300 JB=1,N  !JB is element number to be checked
      IF(L(JB).EQ.0)GO TO 300 !skip if not analyzed
      R1=0.
C
C   Begin checking for overlapping lines
C
      DO 200 KB=1,N  !KB is element number of overlapping line
        DO 150 L2=1,17  !L2 is the line code for KB
      Y1=HI(L2,KB,JB)  !get the overlap factor
      IF(Y1.EQ.0)GO TO 150 !if factor=0 then skip
      E1=EL(L2,KB)  !energy of overlapping line
      L6=LED(L2)
      E2=E(L6,KB)  !energy of edge of overlapping line
      CALL DET(ED,E1,N)  !det. eff.
        T2=FT2(E1)  !conc. average of absorption coef.
      CALL ABSFAC(E2,F1,T2) !f(chi)
      R1=R1+F1*ED*W(JB)*Y1/F(4,JB) !R1 is sum of individual overlaps
  150   CONTINUE
  200 CONTINUE
      W(JB)=XM(JB)-R1  !W contains the corrected intensity
  300 CONTINUE   !and XM still contains the original
  400 CONTINUE   !intensity
      RETURN
      END



      SUBROUTINE PARA(I,J,ZD)
      INCLUDE 'FLUOR.CMN'
C
C  Select parameters for fluorescence correction
C
      CALL YIELD(I,T1,T4,T7)  !get fluorescence yield
      NT=INT(AP(J,I))   !get the parameters for the
      GO TO (100,200,300,400,500,600),NT !particular fluor. correction
  100 ZD=.88*T1  !K exciting K
      RETURN
  200 ZD=3.696*T4 !L exciting K
      RETURN
  300 ZD=.18*T1  !K exciting L
      RETURN
  400 ZD=.75*T4  !L exciting L
      RETURN
```

```
  500 ZD=.01*T1  !K exciting M
      RETURN
  600 ZD=.01*T4  !L exciting M
      RETURN
      END


      SUBROUTINE RDSPEC(IOPT)
C
C   Subroutine to read a spectrum written by TNTVX.
C   This data file contains blocks of two byte words (the least
C   significant part of the number) and blocks of byte integers (the
C   most significant part of the number). These are read and combined
C   in this routine.
C
      INCLUDE 'SPECTM.CMN'
      CHARACTER*10 NAMSP
      INTEGER*2 IARY(2048),IHDR(256)
      BYTE IBYT(2048)
      CLOSE(UNIT=1)
C
C   Enter the file name for the spectrum
C
      TYPE 10
   10 FORMAT('  Spectrum File name? ',$)
      READ(5,15,END=1999) NAMSP
   15 FORMAT(A10)
      IAV=1
C
C     Open the file containing the spectrum.
C
      OPEN(UNIT=1,NAME=NAMSP,TYPE='OLD',FORM='UNFORMATTED',
     1 ACCESS='DIRECT',ASSOCIATEVARIABLE=IAV,RECL=128)
C
C   Read the header of the file (block 1)
C
      READ(1'IAV,IOSTAT=IS,ERR=60)(IHDR(J),J=1,256)
   20 ICH=IHDR(153)  !number of two byte words in file
      ICH=ICH*2/3  !2/3 of words are read as 2-byte
      TYPE 25,(IHDR(J),J=4,13)!types out the file label
   25 FORMAT(1X20A2)
      IAV=2   !data block 2
C
C   Read the 2-byte part of the data
C
      DO 30 I=1,ICH,256 !512 bytes per block
   30    READ(1'IAV,IOSTAT=IS,ERR=60)(IARY(J),J=I,I+255)
C
C   Read the 1-byte part of the data
C
      DO 40 I=1,ICH,512
   40    READ(1'IAV,IOSTAT=IS,ERR=60)(IBYT(J),J=I,I+511)
      DO 50 I=1,ICH
C
```

```
C   Decode 2-byte data
C
          IF(IARY(I).LT.0) THEN !if negative,
         SPEC(I)=IARY(I)+65536 !add 65536
          ELSE
         SPEC(I)=IARY(I)
          END IF
C
C   Decode 1-byte data
C
          IF(IBYT(I).LT.0) THEN !if negative,
         ITEMP=IBYT(I)+256 !add 256
          ELSE
         ITEMP=IBYT(I)
          END IF
C
C   If third byte contains data, add it to SPEC
C
          IF(ITEMP.GT.0) THEN
         SPEC(I)=SPEC(I)+65536*ITEMP
          END IF
   50   CONTINUE
        GO TO 999
   60   TYPE *,'Error number = ',IS !output errors
        TYPE *,'IAV = ',IAV
  999   CLOSE(UNIT=1)   !close spectrum file
        GO TO 2999
 1999   IOPT=-1
 2999   RETURN
        END



      SUBROUTINE ROI(NX)
C
C       Assign the windows around each peak and for the
C       background regions.
C
      INCLUDE 'ROIC.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'SPECTM.CMN'
      DIMENSION EM(10)
      IN=5
C   1 TYPE 10
C  10 FORMAT(' Enter number of background regions desired: ',$)
C     READ(IN,*)NB
    1 TYPE 20
   20 FORMAT(' Enter mean energies for two background points')
        NB=2
      READ(IN,*)(EM(I),I=1,NB)
      DO 100 I=1,NX   !Make sure there are no peaks
             DO 90 J=1,17  !in the background windows.
             FORSIG=4.*S1(EL(J,I))
             FORSIN=EL(J,I)-FORSIG
             FORSIP=EL(J,I)+FORSIG
```

```
            K=1
 30         IF((EM(K).GT.FORSIN).AND.(EM(K).LT.FORSIP)) THEN
              TYPE 40, EM(K), EL(J,I)
 40         FORMAT(' Energy ',F7.3,' interfers with a peak at energy'
   2                ,F7.3)
            TYPE 50
 50         FORMAT(' Do you wish to omit it? ',$)
            READ(IN,60)NY
 60         FORMAT(A1)
               IF(NY.EQ.'Y') THEN
            NB=NB-1
                  DO 70 M=K,NB
 70               EM(M)=EM(M+1)
               END IF
            END IF
           K=K+1
           IF(K.LE.NB) GO TO 30
 90        CONTINUE
100 CONTINUE
    IF(NB.LT.2) THEN
     TYPE 110
110 FORMAT(' You have too few background points - Try again')
    GO TO 1
     END IF
      DO 120 I=1,20
120   CNTS(I)=0.
    NR=NB + NX
    DO 140 I=1,NR   !I is the window number
    IF (I. LE. NB) THEN
      EX=EM(I)   !background window energy
    ELSE
     K= I - NB
     L1 = L(K)
     EX = EL(L1,K)   !peak energy
    END IF
    SK = 1.1775 * S1(EX)  !1/2 FWHM of peak at energy EX
    ELOW(I) = (EX- SK)  !low side of window
    EHI(I) = (EX + SK)  !high side of window
    IL = INT( ELOW(I)*100. + .5) !channel number of ELOW
    IH = INT( EHI (I)*100. + .5) !channel number of EHI
    DO 130 J=IL,IH
130 CNTS(I) = CNTS(I) + SPEC(J) !integrate counts from IL to IH
140 CONTINUE
    RETURN
    END



    FUNCTION S1(E1)
    INCLUDE 'GEOM.CMN'
C
C  Function to compute sigma of a peak of energy E1
C
    S1=SQRT(2500* E1 +Q3)*4.2466E-4
    RETURN
```

```
      END


      SUBROUTINE SETUP(J)
      INCLUDE 'ABSB.CMN'
      INCLUDE 'ATWT.CMN'
      INCLUDE 'BLNK.CMN'
      INCLUDE 'ENER.CMN'
      INCLUDE 'FLUOR.CMN'
      INCLUDE 'ZAFF.CMN'
C
C  Setup matrix correction
C
      DIMENSION U(15),UB(15)
      IB=L(J)**2
      IF(IB.LE.9)GO TO 100
      IB=1
  100 U(J)=E0/E(IB,J)   !overvoltage for element J
      IF(U(J).GE.1.5)GO TO 300  !test if overvoltage too low
      WRITE(6,200)
  200 FORMAT('  OVERVOLTAGE TOO LOW')
  300 L1=L(J)
      E1=EL(L1,J)   !energy of line for element J
      DO 400 I=1,N
      CALL MAC(E1,FA,I)   !get mass absorption coef.
      H(I,J)=FA    !and store them
  400 CONTINUE
      T2=H(J,J)    !absorption coef. for pure element
      E2=E(IB,J)   !edge energy
      CALL ABSFAC(E2,F1,T2)  !get f(chi) for pure element J
      F(1,J)=F1    !and store it
      A3=L(J)-1    !line code minus 1
      GX=5
      IF(L(J).EQ.1) GO TO 500
      IF(L(J).GT.3) GO TO 500
      GX=3.5
  500 DO 800 I1=1,N   !begin checking for fluorescence
      IF(I1.EQ.J)GO TO 800  !skip if same element
      DO 700 IP=1,2   !1 for K lines - 2 for L lines
      E1=EL(IP,I1)   !line energy to test
      L2=IP**2    !edge number
      IF(1.022*E(L2,I1).GE.E0)GO TO 700 !skip if line > E0
      IF(E1.LT.E(IB,J)) GO TO 700 !skip if line < E(IB,J)
      IF(E1.GT.E(IB,J)+GX)GO TO 700 !skip if line > E(IB,J)+GX
      AP(J,I1)=IP+2*A3   !code for fluorescence
C
C       code fluorescence
C       0 none
C       1 K excites K
C       2 L excites K
C       3 K excites L
C       4 L excites L
C       5 K excites M
C       6 L excites M
```

```
C
      UB(I1)=E0/E(L2,I1)  !overvoltage
      DO 600 I=1,N
      CALL MAC(E1,FA,I)   !get absorption coef. for fluor.
      H(I+15,I1)=FA   !and store them
  600 CONTINUE
  700 CONTINUE
  800 CONTINUE
      DO 900 I=1,N
      IF(AP(J,I).EQ.0)GO TO 900  !skip if no fluorescence
      IZ=Z(I)    !Z for exciting line
      JZ=Z(J)    !Z for excited line
      Y2=(UB(I)-1)/(U(J)-1)
      Y2=Y2**1.67
      Y1=WA(JZ)/WA(IZ)*H(J+15,I)/2*Y2
      CALL PARA(I,J,ZD)   !get fluorescence factors
      O(J,I)=ZD*Y1   !fluorescence correction factor
  900 CONTINUE
C
C       Calculate backscatter loss factor R (the loss is 1-R)
C
      U1=U(J)
      IF(U1.LE.10)GO TO 1000
      U1=10
 1000 G3=.00873*U1**3-.1669*U1**2+.9662*U1+.4523
      G4= .002703 *U1 **3 -.05182 *U1 **2 +.302 *U1 -.1836
      P2=.887 -3.44/U1 +9.33/ U1**2- 6.43/U1**3
      DO 1100 I=1,N
      V(I,J)=G3-G4*LOG(P2*Z(I)+25) !this is the R factor
      IZ=Z(I)
C
C       Calculate the stopping power S
C
      S(I,J)=2*IZ/(WA(IZ)*(E0+E(IB,J)))*LOG(583*(E0+E(IB,J))/XJ(IZ))
 1100 CONTINUE
 9999 RETURN
      END



      FUNCTION XJ(IZ)
C
C  Berger-Seltzer J
C
      S19=-.19
      XJ =9.76*IZ+58.5*(IZ**S19) !IZ is atomic number
      RETURN
      END



      SUBROUTINE YIELD(I,T1,T4,T7)
      INCLUDE 'BLNK.CMN'
C
C   Fluorescence yields
```

```
C
      RZ=Z(I)
      ZL=LOG(RZ)
      OM1=(.015+.0327*RZ-6.4E-7*RZ**3)**4
      T1=OM1/(1.+OM1)     !K lines
      T4=EXP(2.946*ZL-13.94)    !L lines
      T7=2.27E-5*Z(I)**2-.001359*Z(I)-.00657 !M lines
      RETURN
      END
```

Files containing common blocks that are used in the INCLUDE

```
C       Variables in common block ABSB
C       F = absorption factors
C       HI = overlap factors
C
      COMMON/ABSB/F(4,15),HI(17,12,12)
```

```
C       Variable in common block ATWT
C       WA = atomic weights
C
      COMMON/ATWT/WA(99)
```

```
C       Variables in common block BLNK and 2-byte integers
C       Z = atomic number
C       Q = valence for each element
C       E0 = beam voltage
C       N = number of elements in standard or unknown
C       NX = number of analyzed elements
C
      INTEGER*2 Z(15),Q(15)
      COMMON/BLNK/E0,N,NX,Z,Q
```

```
C       Variables in common block CONC
C       XC = concentration of each element
C
      COMMON/CONC/XC(15)
```

```
C       Variables in common block DETECT
C       P6 = thickness of Be window in Si detector in cm.
C       P7 = thickness of Si dead layer in Si detector in cm.
C
      COMMON/DETECT/P6,P7
```

```
C       Variables in common block ENER
C       L = line code for x-ray lines (1=Ka,2=La,3=Ma,0=not analyzed)
C       E = edge energies for each element
C       EL = x-ray line energies for each element
C
      INTEGER*2 L(15)
      COMMON/ENER/E(10,15),EL(17,15),L


C       Variables in common block FLUOR
C       AP = code for fluorescence corrections (see SETUP)
C       O = factor in the fluorescence correction
C
      COMMON/FLUOR/AP(15,15),O(15,15)


C       Variables in common block GEOM
C       Q1 = csc(take-off-angle)
C       Q2 = sine of beam incidence angle
C       Q3 = noise factor for peak width calculation
C
      COMMON/GEOM/Q1,Q2,Q3


C       Variables in common block KBKA
C       VB = K-beta/K-alpha ratios (Kb/Ka)
C
      COMMON/KBKA/VB(30)


C       Variables in common block KFAC
C       W = integrated peak intensity for each element
C       XM = relative intensity (k-ratio) for each element
C
      COMMON/KFAC/W(15),XM(15)


C       Variables in common block LINEDG
C       LED = edge number for each of the 17 x-ray lines included
C       in the program.
C
        COMMON/LINEDG/LED(17)
        DATA LED/1,4,9,1,4,4,4,3,3,3,2,2,2,9,8,7,6/
C
C       The x-ray lines are in the following order:
C       Ka,La1,Ma,Kb,La2,Ll,Lb2,Lb1,Lg1,Ln,Lb3,Lg3,Lb4,Mz,Mb,Mg,M2N4
C
```

```
C       Variables in common block ROIC
C       CNTS = integrated counts in a peak window
C       EHI = high energy side of a window
C       ELOW = low energy side of a window
C       NB = number of background regions (currently = 2)
C       NR = total number of regions on a spectrum (background+peaks)
C
      COMMON/ROIC/CNTS(20),EHI(20),ELOW(20),NB,NR



C       Variables in common block SPEC
C       SPEC = number of counts in each channel of a spectrum
C
        INTEGER*4 SPEC
      COMMON/SPECTM/SPEC(2048)



C       H = mass absorption coefficients
C       S = x-ray stopping powers
C       V = R from x-ray loss due to backscatter (1-R)
C
      COMMON/ZAFF/H(30,15),S(15,15),V(15,15)
```

NBS-114A (REV. 2-8C)

U.S. DEPT. OF COMM. **BIBLIOGRAPHIC DATA SHEET** *(See instructions)*	1. PUBLICATION OR REPORT NO. NBS TN1200	2. Performing Organ. Report No.	3. Publication Date July 1984

4. TITLE AND SUBTITLE

A Fortran Version of the Quantitative Energy-Dispersive Electron Beam X-ray Analysis Program FRAME C

5. AUTHOR(S)

R. L. Myklebust, B. B. Thorne

6. PERFORMING ORGANIZATION *(If joint or other than NBS, see instructions)*

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Gaithersburg, Maryland 20899

7. Contract/Grant No.

8. Type of Report & Period Covered

Final

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS *(Street, City, State, ZIP)*

Same as item 6.

10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)*

A Fortran listing of the quantitative electron microprobe analysis routine, FRAME C, is presented. The source code is extensively documented and there are short summaries of the various parts of the program. Examples are also presented to demonstrate the versatility of the program.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

computer program; electron microprobe; energy-dispersive detector; quantitative analysis; x-ray spectra

13. AVAILABILITY

☒ Unlimited

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