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

* 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

<table>
<thead>
<tr>
<th>Z</th>
<th>C</th>
<th>F(X)</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>79</td>
<td>1.0000</td>
<td>0.9619</td>
<td>1.0000</td>
</tr>
<tr>
<td>29</td>
<td>0.0003</td>
<td>0.9799</td>
<td>0.0004</td>
</tr>
</tbody>
</table>
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

EO = 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 ***
EO = 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

<table>
<thead>
<tr>
<th>Z</th>
<th>C</th>
<th>F(X)</th>
<th>K</th>
</tr>
</thead>
<tbody>
<tr>
<td>79</td>
<td>0.3994</td>
<td>0.9619</td>
<td>0.3296</td>
</tr>
<tr>
<td>29</td>
<td>0.6099</td>
<td>0.9799</td>
<td>0.6579</td>
</tr>
</tbody>
</table>

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


IV. Program Listing

FRAME C MAIN PROGRAM

Program for quantitative electron probe microanalysis.
Written by R.L. Myklebust & B. Thorne
National Bureau of Standards
Fortran IV+ for a VAX 11/780 vers. VMS 3.0

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

Add to or create a data file to store the standards information.

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

Main FRAMEC program for standards
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

Open the standards data file if it exists - if it does not exist then create it

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 = ',$)
ACCEPT *,N
TYPE 60
60 FORMAT(' Enter Conc., At.No., Line code, & Valence for each')
DO 70 I=1,N
70 ACCEPT *,XC(I),Z(I),L(I),Q(I)
Z(N+1)=4 !Be for detector window
Z(N+2)=14 !Si for detector dead layer
Z(N+3)=79 !Au for detector
NX=0
DO 80 I=N+1,N+3
L(I)=0
DO 90 I=1,N+3
CALL EDGES(I) !calculate absorption edges
IF(L(I).GT.0) THEN
  NX=NX+1
  CALL LINES(I) !calculate x-ray line energies
LI=L(I)
IF(Z(I).NE.29) GO TO 81
IF(EL(LI,I).LT.1.) THEN
  TYPE 85,Z(I)
  FORMAT(' The line of ',I3,' is less than 1keV')
  GO TO 999
  END IF
IF(E(LI*LI,I).GE.E0) THEN
  TYPE 87,Z(I)
  FORMAT(' The excitation potential of ',I3,' is greater than ',1' than E0')
  GO TO 999
  END IF
END IF
90 CONTINUE
CALL RDSPEC !get spectrum
CALL ROI(NX) !set windows for each element
N3=1 !set number of iterations to 1
CALL OC0EF !calculate overlap factors
CALL BKG !calculate background
CALL OLAPS !correct for overlaps
DO 100 I=1,NX
100 XM(I)=W(I)
CALL MATRIX(QM,N3) !do matrix corrections on standards
C Write standards information into data file.
C
DO 130 I=1,NX
READ(UNIT=10,KEY=Z(I),KEYID=0,IOSTAT=IOS,ERR=110)ZT,LT,XT,QT
110 IF(IOS.EQ.36) THEN
  WRITE(UNIT=10,IOSTAT=IOS,ERR=990)Z(I),L(I),XM(I),Q(I)
  TYPE *,Z(I),L(I),XM(I),Q(I)
ELSE
  TYPE 115,ZT
115 FORMAT(' A file for element ',I3,' already exists - do you'1 ' wish to replace it? ','$)
  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
C SUBROUTINE FRC(NAM, IOPT)
INCLUDE 'BLNK.CMN'
INCLUDE 'CONC.CMN'
INCLUDE 'ENER.CMN'
INCLUDE 'KFAC.CMN'
INCLUDE 'ROIC.CMN'
INCLUDE 'SPECTM.CMN'

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 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 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
  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
I0PT=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 Error conditions for reading, writing and opening files

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)
Compute the area of the Gaussian peak that is integrated within the energy window for each element.

#include 'ROIC.CMN'
E3=EHI(I)  !upper energy of window
E2=ELOW(I)  !lower energy of window
X2=(E2-E7)/SLI(EL)/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)/SLI(EL)/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

This is the FRAME C background calculation

SUBROUTINE BKG
#include 'ABSB.CMN'
#include 'BLNK.CMN'
#include 'CONC.CMN'
#include 'ENER.CMN'
#include 'KFAC.CMN'
#include 'ROIC.CMN'

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
EL=(E2+E3)/2.  !centroid energy of bg window
T2=0.
   DO 10 J=1,N
      CALL MAC(EL,FA,J)
      T2=T2+XC(J)*FA  !concentration average of abs. coef.
10 CONTINUE
CALL DET(ED,EL,N)  !detector efficiency ED
CALL ABSFAC(EL,F1,T2)  !f(chi) F1
T1=ED*F1/EL
X(I)=EO-EL
Y(I)=X(I)/T1
U(I)=X(I)**2
40 CONTINUE
Set up matrix for fit to background

\[ D_1 = X(1) \times U(2) - U(1) \times X(2) \]
\[ X_{K1} = \frac{(Y(2) \times X(1) - Y(1) \times X(2))}{D_1} \]
\[ X_{K2} = \frac{(Y(1) \times U(2) - Y(2) \times U(1))}{D_1} \]

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.
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*XH-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

TYPE *, 'BKG ', T5, G1, GS, ED, F1
CONTINUE
999 RETURN
END

SUBROUTINE COEF(TOA)
INCLUDE 'KBKA.CMN'
INCLUDE 'ATWT.CMN'
INCLUDE 'GEOM.CMN'
INCLUDE 'DETECT.CMN'

Coef. for calculations
Kb/Ka ratios

DATA VB/10*0.,.011,.027,.04,.055,.066,.078,.085,.097,.108
2.,.114,.115,.117,.119,.121,.121,.121,.123,.125/

Table of atomic weights

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.,102.9,106.4,107.9,112.4,114.8,118.8,118.7,121.8,127.6,126.9,131.3
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
8,190.2,192.2,195.1,196.97,200.6,204.4,207.2,209.2,210.2,210.4,210.8,222.0,223.8,226.3,227.2,232.1,231.8,238.7,244.4,243.2,247.4,247.8,247.9,251.0,254.0.

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 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 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 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

19
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*XG(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 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,.27951,.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))
20
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)
      Calculate counts in escape peak
      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
         II=I+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'

      Correction factors in loop
      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
FUNCTION FT2(E1)
INCLUDE 'BLNK.CMN'
INCLUDE 'CONC.CMN'

C
C Conc average of absorb. 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
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
    G5=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. TDGO) 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    Compute incomplete charge correction
C
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 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.

DIMENSION T(3,17)
DATA T/-0.0199726,2.22412,-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(EI,FA,I)
INCLUDE 'BLNK.CMN'
INCLUDE 'ENER.CMN'

C Mass absorption coef.
C EI is the energy of the x-ray line being absorbed. FA is the
C absorption coefficient and I is the index of the absorber.

DIMENSION GJ(3),GK(3),R(10),XD(4,4)

C R is edge jump ratio
DATA R/1.1,.117,1.63,1.1,1.16,1.4,1.621,1.783,1.1/
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(El.LT.E(M1,I)) GO TO 300
200 Ll=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
   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
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.1.0R.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 XM(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
1000 CONTINUE
IF(L(I).GT.0)WRITE(6,960)Z(I),XC(I),F(I,I),XM(I) !analyzed element

1000 CONTINUE
WRITE(6,1020)S3 !output analysis total
1020 FORMAT(1HO,' TOTAL = ',F6.4)
9999 RETURN
END

SUBROUTINE NORM(S3)
INCLUDE 'BLNK.CMN'
INCLUDE 'CONC.CMN'

Normalize concentrations to 100%

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'

DIMENSION WQ(15)

Compute overlap coefficients

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 KL=1,2  !1= self overlap, 2= other overlap
   DO 800 IL=1,N  !Il= analyzed line to be checked
      IF(L(IL).EQ.0)GO TO 800  !skip if unanalyzed element
      L1=L(IL)
   E6=EL(L1,I1)  !line energy of analyzed line
   YD=4*S1(E6)  !4* sigma of analyzed line
   E2=ELLOW(IL+NB)  !low energy of window for Il
   E3=EHI(IL+NB)  !high energy of window for Il
   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
      !Next two lines have the following effect:
      IF((KL.EQ.2).AND.(IL.EQ.J))GO TO 700
      IF((IL.NE.J).AND.(KL.EQ.1))GO TO 700
500 CONTINUE
   IF(L2.EQ.0)GO TO 680  !L2 is a K line
590   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'

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(L2/3)-INT(L2/4)-INT(L2/7))  !electrons per shell

C Overlap for each line
C
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

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 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 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 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
RL=VB(Z(J))
IF(Z(J).LE.30.)GO TO 600

29
RZ = Z(J)
R1 = .115*LOG(RZ) - 2.3 ! compute Kb/Ka for elements (Z=30)

S(2,J) = V2 ! L a1
S(3,J) = V3 ! M a
S(4,J) = R1/(1-R1)*V1 ! K b
S(5,J) = .1*V2 ! L a2
S(6,J) = .04*V2 ! L 1
S(7,J) = V2*(.2808-.0016*Z(J)) ! L b2
S(8,J) = V5 ! L b1
S(9,J) = .15*V5 ! L g1
S(10,J) = .02*V5 ! L n
S(11,J) = .16*V4 ! L b3
S(12,J) = .06*V4 ! L g3
S(13,J) = .10*V4 ! L b4
S(14,J) = .06*V3 ! M z1
S(15,J) = .5*V3*U(9)/U(10) ! M b
S(16,J) = .05*V3*U(8)/U(10) ! M g
S(17,J) = .01*V3*U(7)/U(10) ! M 2 N 4

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 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,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 H1(I2,J,J1) = 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 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 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 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
SUBROUTINE RDSPEC(IOPT)
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
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

Open the file containing the spectrum.
OPEN(UNIT=1,NAME=NAMSP,TYPE=' OLD',FORM=' UNFORMATTED',
1 ACCESS=' DIRECT',ASSOCIATEVARIABLE=IAV,RECL=128)
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
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
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 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 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 Assign the windows around each peak and for the
C background regions.
C
INCLUDE 'ROIC.CMN'
INCLUDE 'ENER.CMN'
INCLUDE 'SPECTM.CMN'
DIMENSION EM(IO)
IN=5
C 1 TYPE 10
C 10 FORMAT( ' Enter number of background regions desired: ',$)
READ(IN,*)NB
1 TYPE 20
20 FORMAT( ' Enter mean energies for two background points' )
NB=2
READ(IN,*)(EM(I),I=1,NB)
DO 100 I=1,NX !Make sure there are no peaks
DO 90 J=1,17 !in the background windows.
FORSIG = 4.*S1(EL(J,I))
FORSIN = EL(J,I) - FORSIG
FORSIP = EL(J,I) + FORSIG
90 CONTINUE
100 CONTINUE
K=1
30 IF((EM(K).GT.FORSIN).AND.(EM(K).LT.FORSIP)) THEN
   TYPE 40, EM(K), EL(J,I)
40 FORMAT(' Energy ',F7.3,' interferes with a peak at energy' ,F7.3)
   TYPE 50
50 FORMAT(' Do you wish to omit it? ',$,)
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
SUBROUTINE SETUP(J)
INCLUDE 'ABSB.CMN'
INCLUDE 'ATWT.CMN'
INCLUDE 'BLNK.CMN'
INCLUDE 'ENER.CMN'
INCLUDE 'FLUOR.CMN'
INCLUDE 'ZAFF.CMN'

C Setup matrix correction

DIMENSION U(15),UB(15)
IB=L(J)**2
IF(IB.LE.9)GO TO 100
IB=1
100 U(J)=EO/E(IB,J) ! overvoltage for element J
IF(U(J).GE.1.5)GO TO 300 ! test if overvoltage too low
WRITE(6,200)
FORMAT(' OVERVOLTAGE TOO LOW')
200
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 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

35
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 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
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

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

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

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

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

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

L = line code for x-ray lines (1=Ka, 2=La, 3=Ma, 0=not analyzed)
E = edge energies for each element
EL = x-ray line energies for each element

INTEGER*2 L(15)
COMMON/ENER/E(10,15), EL(17,15), L

Variables in common block FLUOR

AP = code for fluorescence corrections (see SETUP)
O = factor in the fluorescence correction

COMMON/FLUOR/AP(15,15), O(15,15)

Variables in common block GEOM

Q1 = csc(take-off-angle)
Q2 = sine of beam incidence angle
Q3 = noise factor for peak width calculation

COMMON/GEOM/Q1, Q2, Q3

Variables in common block KBKA

VB = K-beta/K-alpha ratios (Kb/Ka)

COMMON/KBKA/VB(30)

Variables in common block KFAC

W = integrated peak intensity for each element
XM = relative intensity (k-ratio) for each element

COMMON/KFAC/W(15), XM(15)

Variables in common block LINEDG

LED = edge number for each of the 17 x-ray lines included in the program.

COMMON/LINEDG/LED(17)
DATA LED/1, 4, 9, 1, 4, 4, 4, 3, 3, 3, 2, 2, 9, 8, 7, 6/

The x-ray lines are in the following order:
Ka, La1, Ma, Kb, La2, Ll, Lb2, Lbl, Lg1, Ln, Lb3, Lg3, Lb4, Mz, Mb, Mg, M2N4
Variables in common block ROIC
CNTS = integrated counts in a peak window
EHI = high energy side of a window
ELOW = low energy side of a window
NB = number of background regions (currently = 2)
NR = total number of regions on a spectrum (background+peaks)

COMMON/ROIC/CNTS(20),EHI(20),ELOW(20),NB,NR

Variables in common block SPEC
SPEC = number of counts in each channel of a spectrum

INTEGER*4 SPEC
COMMON/SPECTM/SPEC(2048)

H = mass absorption coefficients
S = x-ray stopping powers
V = R from x-ray loss due to backscatter (1-R)

COMMON/ZAFF/H(30,15),S(15,15),V(15,15)
4. TITLE AND SUBTITLE
A Fortran Version of the Quantitative Energy-Dispersive Electron Beam X-ray Analysis Program FRAME C

5. AUTHOR(S)
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6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)
National Bureau of Standards
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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

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