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NBSGSC—A FORTRAN Program for Quantitative X-ray Fluorescence Analysis

G. Y. Tao, P. A. Pella, and R. M. Rousseau

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NBSGSC - A FORTRAN Program For Quantitative X-Ray Fluorescence Analysis

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ABSTRACT

A FORTRAN program (NBSGSC) was developed for performing quantitative analysis of bulk specimens by x-ray fluorescence spectrometry. This program corrects for x-ray absorption/enhancement phenomena using the comprehensive alpha coefficient algorithm proposed by Lachance (COLA). NBSGSC is a revision of the program ALPHA and CARECAL originally developed by R.M. Rousseau of the Geological Survey of Canada. Part one of the program (CALCO) performs the calculation of theoretical alpha coefficients, and part two (CALCOMP) computes the composition of the analyte specimens. The analysis of alloys, pressed minerals, and fused specimens can currently be treated by the program. In addition to using measured x-ray tube spectral distributions, spectra from seven commonly used x-ray tube targets could also be calculated with an NBS algorithm included in the program. NBSGSC is written in FORTRAN IV for a Digital Equipment Corporation (DEC PDP-11/23) minicomputer using RL02 firm disks and an RSX 11M operating system.

Key words: Alpha coefficients; comprehensive algorithm; fundamental parameters; interelement corrections; program; quantitative analysis; x-ray.

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TABLE OF CONTENTS

I. INTRODUCTION

NBSGSC was developed in response to a need in the X-ray spectrometry community for a generally available fundamental parameter program for correction of interelement (matrix) effects in quantitative X-ray fluorescence spectrometry. This program was designed for X-ray analysis of samples where direct X-ray tube excitation is employed. Although there are fundamental parameter programs available through commercial suppliers, they are essentially proprietary documents. Probably the best known fundamental parameter program generally available to the user is the Naval Research Laboratories' NRLXRF (1). This program, however, requires extensive computer capabilities and is not subject to general modification by the user. NBSGSC was written to run on present-day minicomputers such as a DEC PDP* 11/23 system. Because the entire source program information is well-documented in this publication, any modification by the user should be possible for particular applications. However, the authors specifically decline responsibility for any error arising from modifications made and/or improper use of these algorithms.

Another impetus for developing NBSGSC was the opportunity to evaluate a recent comprehensive algorithm proposed by Lachance (2) which we call COLA. This algorithm uses a theoretical alpha coefficient approach to the correction of matrix effects unlike most other fundamental parameter programs. In addition, we also desired to test a new NBS algorithm (3) for calculation of X-ray tube spectral distributions required in fundamental parameter methods when the source of excitation of a specimen is an X-ray tube.

To test the COLA algorithm, we obtained a computer program developed by R. M. Rousseau of the Geological Survey of Canada (GSC). This program was extensively modified at NBS and ultimately evolved into what we will now refer to as the NBSGSC program.

The modifications are summarized as follows:

(1) Instead of calculating α-coefficients for alloys (element system), minerals (oxide system) and fused disc specimens in separate programs, these options were combined into a single program.

(2) Two options now exist for X-ray tube spectral distributions. Either measured X-ray spectral distributions from the literature or distributions calculated from the NBS algorithm for seven commonly used X-ray tubes at any voltage can be employed.

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*Disclaimer - In order to adequately describe materials and experimental procedures, it was occasionally 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.

(3) Most of the fundamental parameters required for calculating alpha coefficients such as mass absorption coefficients, fluorescence yields, jump ratio, analyte line wavelength, absorption edge wavelength, are either computed or stored in the program to minimize data input by the user.

(4) For calculating mass absorption coefficients, either the algorithm of Heinrich or the necessary table values from Thinh and Leroux can be selected. The table values for Thinh and Leroux are stored in a permanent datafile.

(5) When analyzing specimens, known concentrations of any unanalyzed elements can now be entered at fixed concentrations.

(6) A dead-time correction has been incorporated in the program.

(7) Four types of calibration curves can be selected for system calibration.

(8) One of three sample preparation conditions can be chosen when fusing specimens to allow greater flexibility in sample-to-flux ratios used in various laboratories.

(9) If the results of analysis are to be compared with previously known or "true" values for the analyte specimens, the program will output absolute and relative errors.

An evaluation of the COLA algorithm has been performed and is the subject of a publication (4) where results were intercompared with those obtained with NRLXRF for typical alloys, and minerals both in the pressed powder and fused disc form. The general form of the COLA expression is:

$$C_i = R_i(1+\Sigma_j \alpha'_{ij} C_j + \Sigma_j \Sigma_k \alpha'_{ijk} C_j C_k) \qquad (1)$$

where C_i is the analyte weight fraction, and $C_{j,k}$ are the corresponding weight fraction of elements j and k, respectively. R_i is the analyte X-ray intensity relative to the pure analyte. The coefficient α'_{ij} quantifies the effect of element j on i and is equal to

$$\alpha'_{ij} = \alpha_1 + \frac{\alpha_2 C_m}{1+\alpha_3(1-C_m)} \qquad (2)$$

where $C_m = C_j + C_k + \cdots$

The concept of "crossed" coefficients introduced by Claisse-Quintin (5) is retained where α'_{ijk} is defined as follows:

$$\alpha'_{ijk} = \frac{1}{C_j C_k}\left[\frac{C_i}{R_i} - (1+\alpha'_{ij}C_j+\alpha'_{ik}C_k)\right] \qquad (3)$$

Both α'_{ij} and α'_{ijk} are primed to indicate that the coefficients represent variables which in practice, however, are treated as changing predictably within relatively narrow limits. The three constants α_1, α_2, and α_3 in equation 2 are calculated from hypothetical binary samples. For example, in alloy systems, α_1 is the value of the coefficient near the $C_i = 1.0$ limit (in practice computed at $C_i = 0.999$; $C_j = 0.001$). The value for α_2 is the range within which α'_{ij} will vary when the concentration of the analyte decreases to the $C_i = 0.0$ limit (in practice computed from two binaries $C_i = 0.001$, 0.999; $C_j = 0.999$; 0.001). The α_3 coefficient expresses the rate with which α'_{ij} is made to vary hyperbolically within the two stated limits. In practice, it is generally computed from three binaries where $C_i = 0.001$, 0.5, 0.999; $C_j = 0.999$, 0.5, 0.001. Since α_3 can take on positive, zero, or negative values, α'_{ij} can be computed for the entire composition range from $C_i = 1.0$ to 0.0. The α'_{ijk} coefficients are included to compensate for the fact that the total interelement correction cannot be strictly represented by a sum of binary matrix effects. A value for α'_{ijk} calculated from equation 3 ($C_i = 0.30$, $C_j = 0.35$, $C_k = 0.35$) where the binary α'_{ij} and α'_{ik} are calculated at the $C_i = 0.30$, $C_{j,k} = 0.70$ level can generally be used to represent the entire α'_{ijk} array.

For the multi-element assay of alloys, all the coefficients in equation 1 are calculated. For such specimens as cements, α_3 is nearly equal to zero, so that α'_{ij} in equation 2 can be simplified to

$$\alpha'_{ij} = \alpha_1 + \alpha_2 C_m . \qquad (4)$$

Note that α'_{ij} here is equivalent to that coefficient in the Claisse-Quintin model and equation 2 now reduces to the Claisse-Quintin expression. Hypothetical binary standards where $C_i = 0.2$ and 0.8, and $C_j = 0.8$ and 0.2 are generally used to calculate α'_{ij} values.

For fused specimens, another simplification in equation 2 can be made because the concentration of the flux is by far the major constituent and can be held relatively constant. In this case α_2, α_3, and α'_{ijk} are approximately zero, so that α'_{ij} reduces to α_{ij} in the conventional Lachance-Traill (6) expression. Hypothetical binary standards are used to calculate α_{ij} values where C_i equals the mid-range of the concentrations in the analyte.

We propose that NBSGSC is suitable for routine analysis of alloys, and minerals both as powders, and as fused specimens. Once the theoretical alpha coefficients are calculated and saved in a data file, the user can employ them at any time along with measured X-ray intensity data on standards and unknowns to obtain concentrations. Theoretical alpha coefficients only provide the general relationship of matrix influences on the analyte, and user-defined real standards are used to rescale it for matching experimental reality. Therefore, appropriate standards are very important for obtaining good results as is the case with other fundamental parameter methods [1,7]. Since NBSGSC is generally written in Standard FORTRAN IV, it should be readily adaptable to most minicomputers in laboratories which use X-ray fluorescence spectrometry.

To achieve optimum analytical results, it should be recognized by the user that accurate net x-ray intensities need to be measured. Corrections to measured x-ray intensities for background, blanks, x-ray line overlaps, detector dead-time,and spectral artifacts such as sum and escape peaks, should always be carefully considered.

II. PROGRAM STRUCTURE

NBSGSC is divided into two separate programs (CALCO and CALCOMP*) where each program consists of a main program and a series of subprograms linked to the main program as shown in Figures 1 and 2. The list of symbols and permanent data files used in programs CALCO and CALCOMP are presented in appendix 2.

In CALCO, a subroutine TUBDAT along with subroutines CTNLIN, CHALIN, INFTGT and datafile TGTWR.DAT are used mainly to perform the calculation of the X-ray tube spectral distribution. This requires input of the X-ray tube target, voltage, take-off angle, Be window thickness, and the ending wavelength of the continuum. The spectral distribution calculation is based on an NBS algorithm proposed by Pella and Feng [3], which utilized experimental electron microprobe data obtained under various conditions. The calculation of the X-ray intensities for both the continuum and characteristic lines (KA, KB, LA1, LB1) from the X-ray tube are performed in CTNLIN and CHALIN respectively, and intensities for the other characteristic lines (LB2, LB3, LB4, LG1 = LY1, LG2 = LY2, LG3 = LY3, LL) are obtained from the intensity ratios of the lines to the LA1 line tabulated in the literature [8].

There are two real functions, named MAC and MACFUN, each of which could be chosen for computing mass absorption coefficients. When using the function MAC, the mass absorption coefficients are calculated from the algorithm of Heinrich [9] using the general relation

$$\mu = C\lambda^n \tag{5}$$

where λ is the wavelength in angstroms and the coefficient C is calculated by a least-squares fit. Parameters required in the function MACFUN using the general equation of Thinh and Leroux [10], that is,

$$\mu = C\, E_{ab}\, \lambda^n \tag{6}$$

where E_{ab} is the absorption edge energy (keV), however, are all stored in the direct-access datafile MACPRM.DAT. MACFUN requires more time to calculate mass absorption coefficients than the function MAC.

The wavelengths of analyte lines (KA, KB or LA1, LB1 or LB2), the corresponding wavelengths of the absorption edges (for K or LII or LIII shell) and the corresponding X-ray fluorescent yields (for K or LII or LIII shell) are computed in Subroutines CHAWV, ABSEDG, and YIELD, respectively, by means of empirical fits. The jump ratio values for the K or LIII shell, however, are stored in Subroutine JUMRAT. The atomic fraction of an analyte in an oxide compound is calculated in the Subroutine AFIOX.

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*Disclaimer - CALCOMP is an acronym for calculation of composition and is not intended to refer to the commercial company by the same name.

FIGURE 1. STRUCTURE OF PROGRAM CALCO

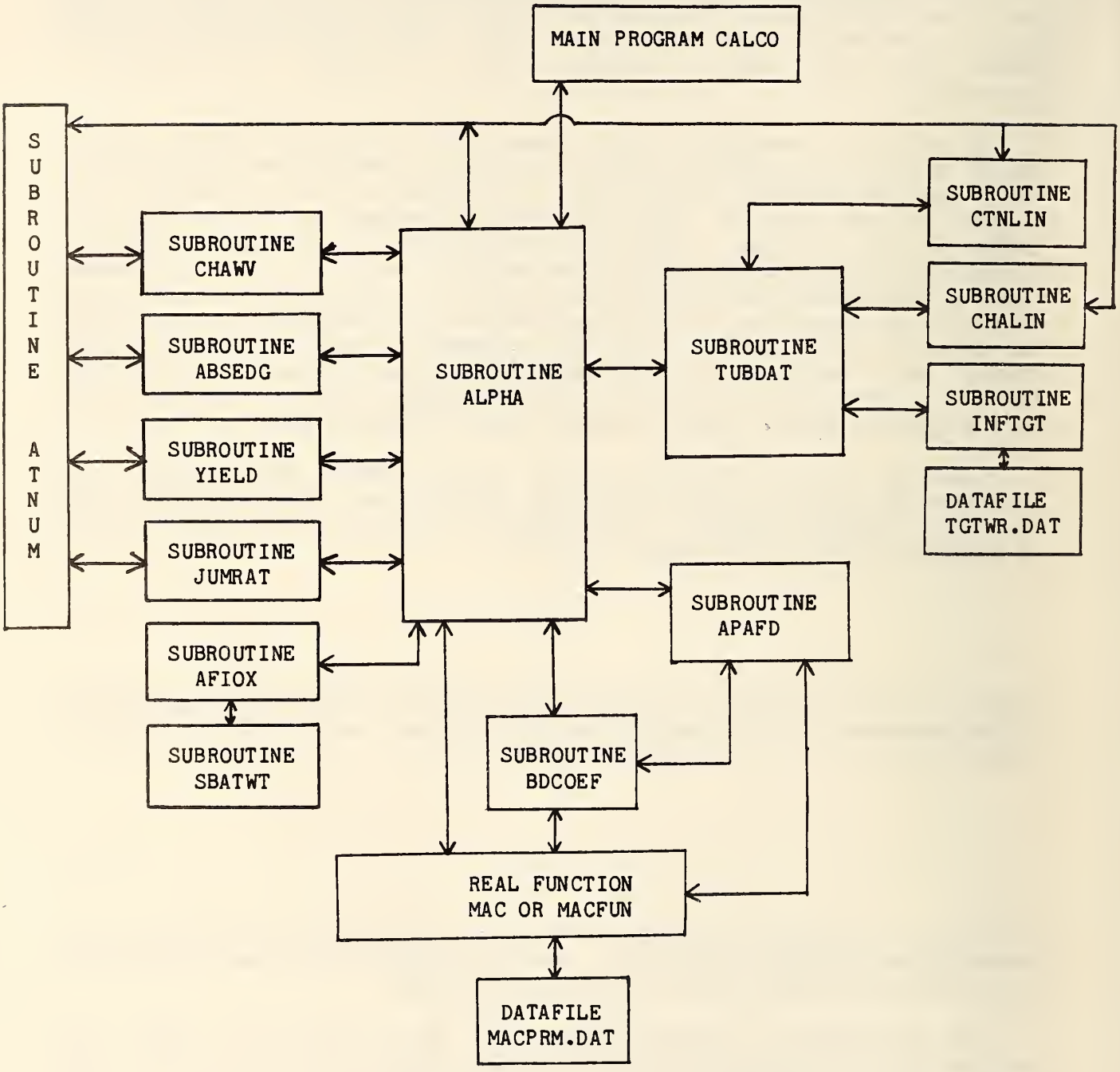
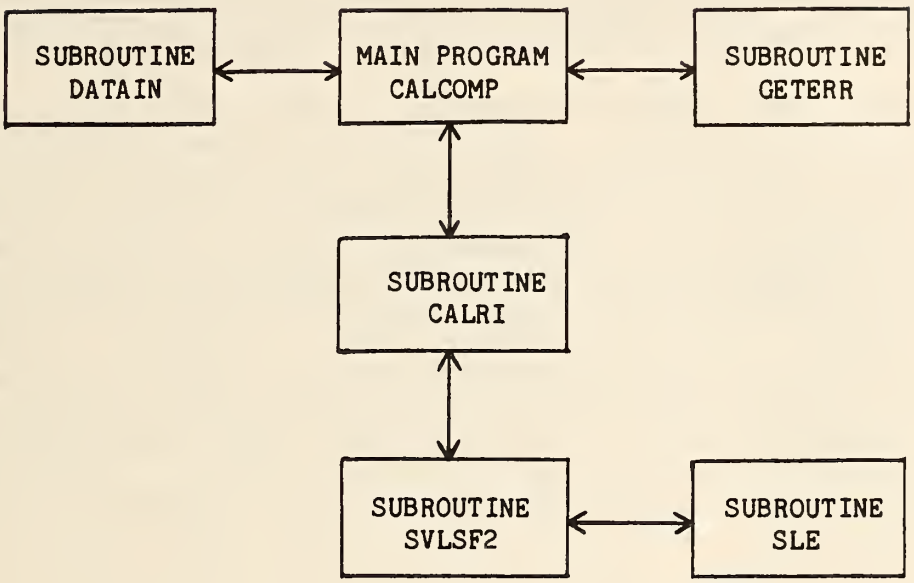


FIGURE 2. STRUCTURE OF PROGRAM CALCOMP



Subroutine ALPHA, along with subroutines BDCOEF and APAFD, completes the major calculation of alpha coefficients, which are α_1, α_2, α_3, and α'_{ijk} for an element system, α_1, α_2, and α'_{ijk} for an oxide system, or α_1 for a fused disc system. Calculated alpha coefficients can be saved in a sequential-access datafile created by the main program CALCO if desired. Frequently used common subroutines, ATNUM and SBATWT provide the atomic number and atomic weight, respectively, when the chemical symbol of an element is given.

In CALCOMP, input data are required for alpha coefficients, intensities and concentrations of standards, and intensities of unknowns using the subroutine DATAIN. After relative intensities of the standards are calculated, subroutine CALRI calls subroutines SVLSF2 and SLE to obtain a least-square fit for the calibration curve (R_i^s versus I_i^s), and then from this calibration curve relative intensities for unknowns are computed and sent back to the main program CALCOMP where iterations proceed to obtain the final concentrations of unknowns. Subroutine GETERR is used, if desired, to compare the observed results with other previously known values for the unknowns. The options for selecting different analysis systems, entering known concentrations of unanalyzed elements as fixed concentrations, dead time correction, different calibration curves, and for using different standards such as multi-element or pure element standards are also provided in the program CALCOMP.

III. OPERATING PROCEDURE

A menu procedure for operating the programs CALCO and CALCOMP is followed where the user answers a question, selecting the appropriate answer among the ones provided, and enters the required data. This is illustrated by the flowcharts in Figures 3 and 4. Examples of the menus are shown in appendix 3. For ensuring proper execution of the program, the following additional comments are made to the user.

For CALCO (refer to figure 3)

(1) In step 2, if an oxide system is selected for analysis, and the user wishes to add LOI (loss of ignition) as an analyte, α_{LOI} is computed assuming the hypothetical compound CO_3 as an approximation to CO_2 plus H_2O. (See example in Appendix 3.3A). If the fused disc system is selected, α_{LOI} is automatically calculated at the 25% level and stored by the program.

(2) The maximum number of analytes the program can handle in step 2 is 12. But in a fused disc analysis the actual number is 12 plus 1 because LOI is already taken into account.

(3) It is recommended that names of the analytes are entered in the order of increasing atomic number in step 4. For an element system, each name occupies three spaces. The first two for the chemical symbol of the analyte, the third one as a blank space such as FE# or V## where # represents a blank space. For an oxide or fused disc system, a special format for the name is required to automatically calculate the atomic fraction of the element in its oxide. In this case, each name occupies six spaces. The first two for the chemical symbol of analyte, the third one for number of analyte atoms in the corresponding oxide, the fourth one for the chemical symbol of oxygen, the fifth one for the number of oxygen atoms in the oxide, and the sixth one as a blank space for example MG101#P#205#FE203# etc.

(4) If the user selects measured X-ray tube spectral data in step 12, then a datafile should be created by EDT before running the program. The data should be in the following order:

1. Wavelengths of the continuum from the short wavelength limit to the ending wavelength in intervals of 0.02 A.

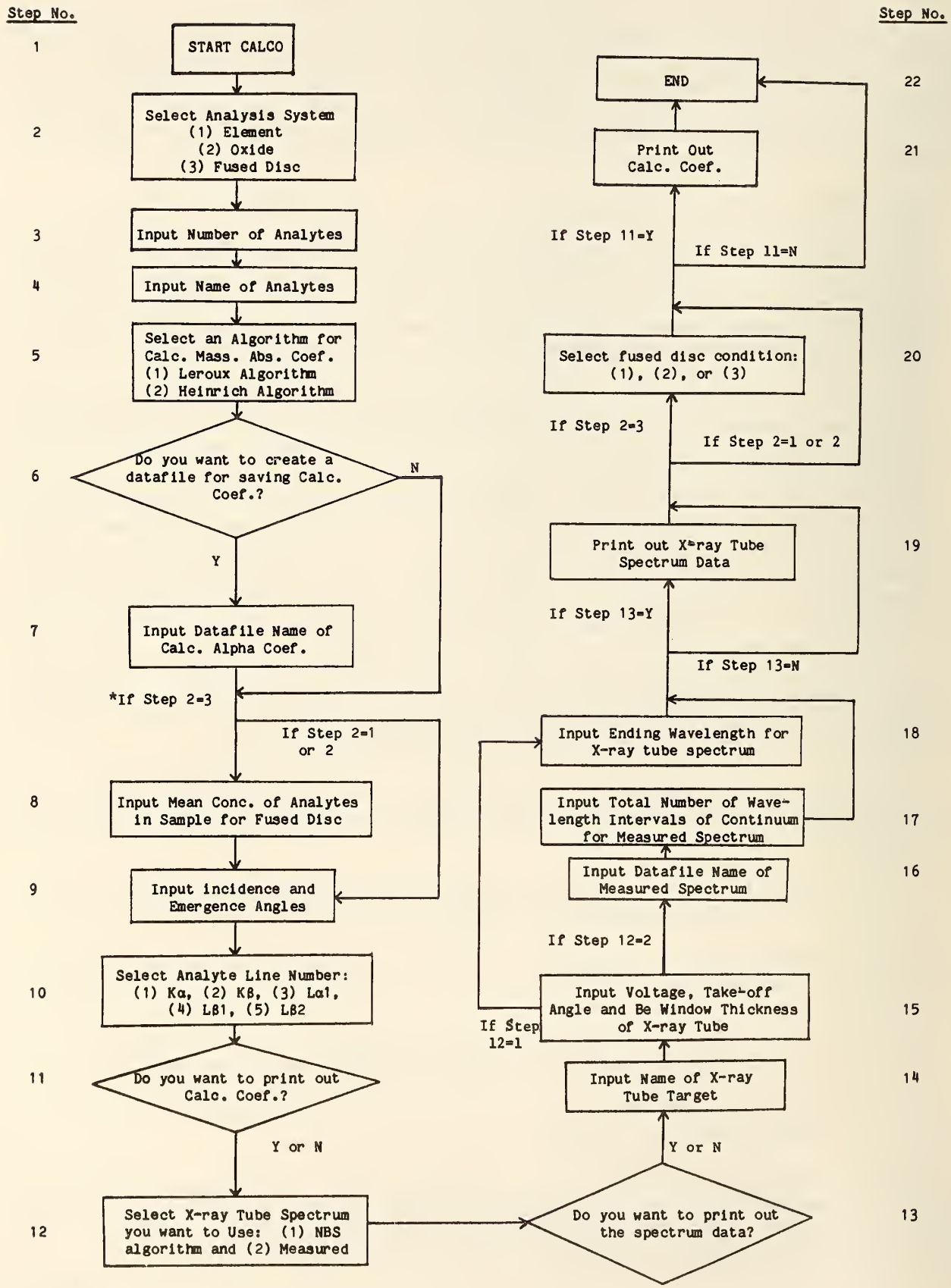
2. The integral intensities of the continuum for each wavelength interval.

3. The wavelengths of the X-ray tube characteristic lines in order of KA, KB, LA1, LB1, LB2, LB3, LB4, LG1, LG2, LG3, and LL.

4. The intensities of the X-ray tube characteristic lines in the same order as 3 above.

Table 1 gives an example of a datafile named SDXT75.W45, containing measured spectral data for the tungsten target at 45 kV published in 1975 [11]. The total number of wavelength intervals (maximum number = 300) of the continuum for the measured spectrum is also entered in step 17.

FIGURE 3. FLOWCHART FOR PROGRAM CALCO



*This means if option 3 is selected in Step 2, etc.

FIGURE 4. FLOWCHART FOR PROGRAM CALCOMP

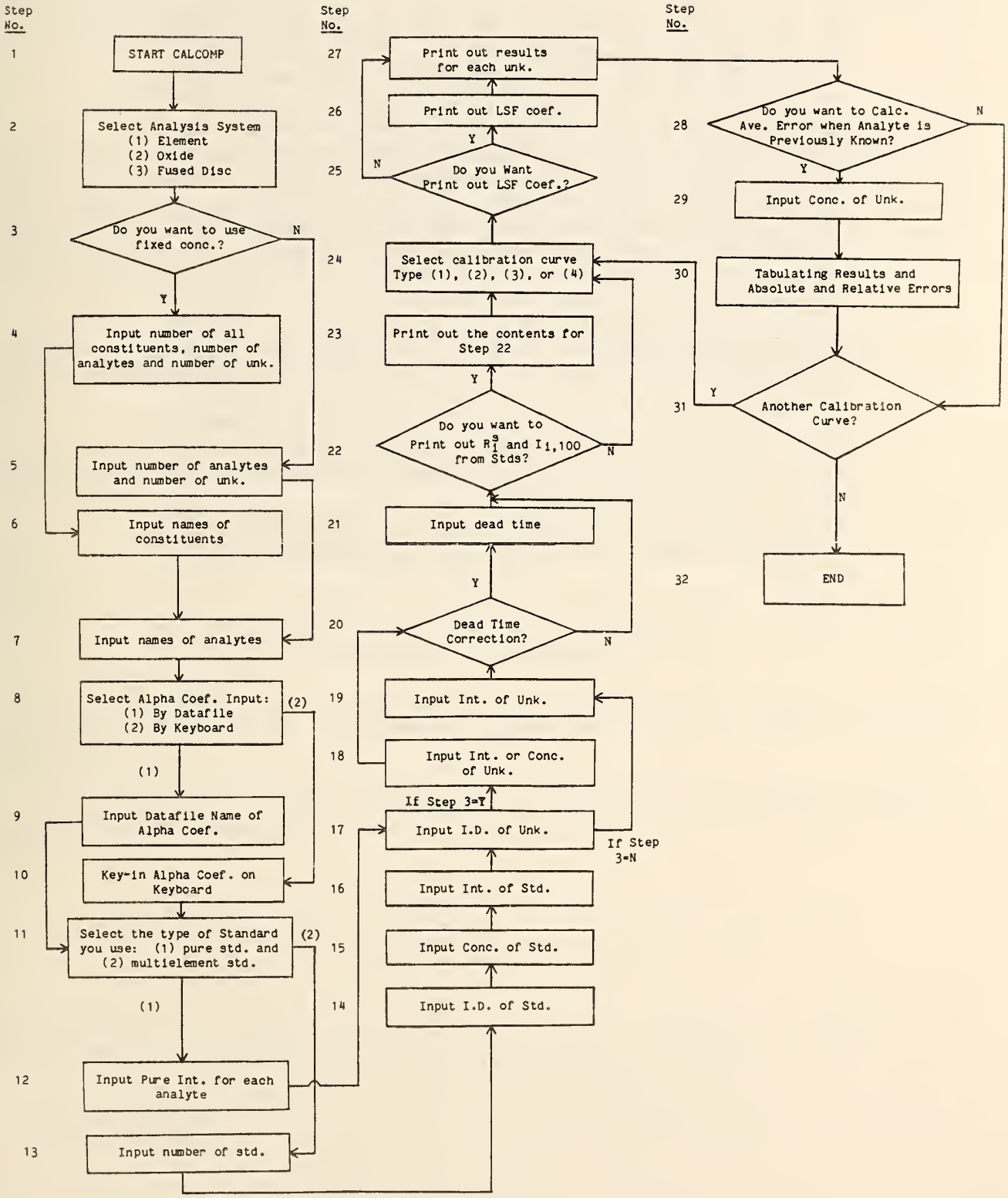


Table 1. The Contents of Datafile SDXT75.W45 as an Example of Measured X-ray Tube Spectral Data

```
.27,.29,.31,.33,.35,.37,.39,.41,.43,.45,.47,.49,.51,.53
.55,.57,.59,.61,.63,.65,.67,.69,.71,.73,.75,.77,.79,.81
.83,.85,.87,.89,.91,.93,.95,.97,.99,1.01,1.03,1.05,1.07
1.09,1.11,1.13,1.15,1.17,1.19,1.21,1.23,1.25,1.27,1.29
1.31,1.33,1.35,1.37,1.39,1.41,1.43,1.45,1.47,1.49,1.51
1.53,1.55,1.57,1.59,1.61,1.63,1.65,1.67,1.69,1.71,1.73
1.75,1.77,1.79,1.81,1.83,1.85,1.87,1.89,1.91,1.93,1.95
1.97,1.99,2.01,2.03,2.05,2.07,2.09,2.11,2.13,2.15
2.17,2.19,2.21,2.23,2.25,2.27,2.29,2.31,2.33,2.35,2.37
2.39,2.41,2.43,2.45,2.47,2.49,2.51,2.53,2.55,2.57,2.59
0.0,4.4,13.1,20.9,27.7,32.7,35.7,37.8,39.0,39.3,39.2,38.8,38.2
37.4,36.6,35.7,34.8,34.0,33.1,32.2,31.4,30.4,29.6,28.8
28.0,27.2,26.3,25.6,24.8,24.0,23.4,22.6,21.9,21.2,20.6
20.0,19.4,19.1,18.9,18.9,19.3,19.6,19.0,18.4,18.0,17.4
17.0,17.6,21.1,21.4,20.8,20.2,19.7,19.1,18.5,18.0,17.5,17.0
16.5,16.0,15.5,15.0,14.6,14.1,13.7,13.3,12.9,12.5,12.2
11.8,11.4,11.1,10.8,10.4,10.2,9.8,9.6,9.3,9.0,8.7,8.4,8.2
7.9,7.7,7.4,7.2,7.0,6.7,6.5,6.2,6.0,5.8,5.6,5.4,5.2,5.0
4.8,4.7,4.5,4.4,4.2,4.0,3.8,3.7,3.6,3.5,3.3,3.2,3.1,3.0
2.8,2.7,2.6,2.5,2.4,2.3,2.2
0.0,0.0,1.4776,1.2818,1.2454,1.2627,1.3016,1.0986,1.0686
1.062,1.6782,0.0,0.0,535.,331.5,153.,50.,50.,61.,9.25
6.95,18.2
```

(5) If the NBS algorithm is selected for calculating the X-ray tube spectral distribution in step 12, one of the following seven X-ray targets can be chosen: Sc, Cr, Mo, Rh, Ag, W, or Au.

(6) When the Cr target X-ray tube is used where Cr and Mn are among the analytes, an aluminum filter, 0.081 g/cm^2 thick is employed and the primary spectrum is corrected by the absorption of the filter for these two analytes automatically in the program.

For program CALCOMP (refer to figure 4).

(1) If you answer 'Y' in step 3, that means known concentrations of unanalyzed elements could be entered as fixed concentrations, and 'NUMBER OF ALL CONSTITUENTS' in step 4 means the sum of the number of analytes and unanalyzed elements. In step 18 when asked for the input of intensities or concentrations of unknowns, the fixed concentrations (weight fraction) should be entered for unanalyzed elements while intensities are entered for the analytes.

(2) In steps 6 or 7, each name occupies eight spaces and the name has no defined function meaning, so that TI######V#######FE###### or LOI#####MGO#####SIO2####P2O5#### are all correct (see example in appendix 3).

(3) If the alpha coefficients in step 8 are entered via '2-KEYBOARD', the order to key in alpha coefficients is as follows:

1. The coefficients for the analytes are entered in the same order as the input names of the analytes in steps 6 or 7.

2. For each analyte, the order of entering coefficients is α_1, α_2, α_3, and α'_{ijk}, as listed in the tabulation of alpha coefficients where blank spaces should be replaced by zero.

In appendix 3.1A is an example of the tabulation of alpha coefficients for the CR-FE-NI system. An example of how these data are keyed in appears in appendix 3.1B.

(4) Calculated relative intensities of standards in step 22 are computed using the COLA algorithm:

$$R_i^s = C_i/[1+\sum_j(\alpha_1 + \frac{\alpha_2 \cdot C_m}{1+\alpha_3(1-C_m)}) \cdot C_j + \sum_j \sum_k \alpha'_{ijk} \cdot C_j \cdot C_k]$$

and intensities corresponding to the pure analyte element are computed from multi-element standards using the equation: $I_{i,100} = I_I^s/R_i^s$

(5) In step 24, four choices of calibration curves may be selected by the user and are:

1. straight line: Y = AO+A1*X
2. quadratic line: Y = AO+A1*X+A2*X*X
3. straight line constrained to zero intercept: Y = A1*X
4. quadratic line constrained to zero intercept: Y = A1*X+A2*X*X

In many cases, calibration curve 4 seems to partially compensate for inaccuracies in fundamental parameters used in the calculation of theoretical alpha coefficients especially over a wide range of analyte composition, and better results have been observed. However, when the concentrations of the unknowns are out of the range of the standards, it is suggested that the other calibration curves listed above be used to check for consistency in the results. The extrapolation provided by the quadratic line can sometimes give large errors.

When only one multielement standard is available, calibration curve 3 is the only option used by CALCOMP. At least two multielement standards are required for calibration curve 1 or 4, while three are required for calibration curve 2.

(6) In the final printout of the results for each unknown, 'R' is the relative intensity 'C' is the concentration in weight percent, and 'L' is the number of iterations.

(7) The convergence criterion to be met for all analytes in the program is 0.01%. If the number of iterations exceeds 10 and convergence is still not reached, the program will pause and print out the warning message "NO. OF ITERATION >10'. One could still print out the results at this stage by keying in the command 'RESUME', at which point the results of the last iteration are printed out, and the program automatically begins to process the next unknown sample. In practice, convergence is usually obtained in three to seven iterations.

The examples given in appendix 3 illustrate the program input and output structures for running the different analysis schemes. For more efficient operation, especially for routine applications, it is recommended that a command file be created by the user which will contain the answers to the menu questions and all required input data in the format specified in CALCO and CALCOMP, prior to execution of the program. Use of a command file in this way is especially advantageous when few changes in input data need to be made as different specimens are analyzed.

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Appendix 1: Listing of CALCO and CALCOMP Programs

```
      PROGRAM CALCO
C
C       THIS IS A REVISION OF VERSION 1 OF A FUNDAMENTAL PARAMETER
C      COMPUTER PROGRAM FOR CORRECTION OF INTERELEMENT EFFECTS FOR
C      QUANTITATIVE X-RAY SPECTROMETRY. THE ORIGINAL PROGRAM WAS
C      WRITTEN BY R.M.ROUSSEAU OF THE GEOLOGICAL SURVEY OF CANADA
C      (GSC) AND CONTAINS THE PROGRAMS ALPHA AND CARECAL WHICH WERE
C      EXTENSIVELY MODIFIED AT NBS. THE NBSGSC PROGRAM CONTAINS THE
C      COMPREHENSIVE LACHANCE ALGORITHM(COLA) FOR CORRECTION OF INTER-
C      ELEMENT EFFECTS.
C       CALCO IS A REVISION OF ALPHA FOR CALCULATING THEORETICAL ALPHA
C      COEFFICIENTS, AND CALCOMP IS A REVISION OF CARECAL FOR CALCULA-
C      TING CONCENTRATIONS IN ANALYTE SPECIMENS.
C
C      OVERLAY STRUCTURE OF CALCO :
C        MAIN PROGRAM-----CALCO
C        SUBROUTINE-------ALPHA,APAFD,ATNUM,CHAWV,ABSEDG
C                         JUMRAT,YIELD,AFIOX,BDCOEF,TUBDAT
C                         CINLIN,INFTGT,CHALIN,SBATWT
C        REAL FUNCTION----MAC,MACFUN
C        DATAFILE---------TGTWR.DAT,MACPRM.DAT
C                       *
C      AUTHORS: G.Y. TAO  AND P.A. PELLA          DATE: 04-SEP-1984
C        CENTER FOR ANALYTICAL CHEMISTRY, NATIONAL BUREAU OF STANDARDS
C        GAITHERSBURG MD 20899 U.S.A.
C              AND R.M.ROUSSEAU
C        GEOLOGICAL SURVEY OF CANADA, OTTAWA, CANADA K1A-0E8
C
C      * GUEST RESEARCHER FROM SHANGHAI INSTITUTE OF CERAMICS,
C        ACADEMIA SINICA, THE PEOPLE'S REPUBLIC OF CHINA
C
      DIMENSION IELE(12),NE(12),NO(12),A1(12,12),A2(12,12),
     + A3(12,12),AIJK(12,12,12),IDATE(5),ITIME(4),NAMFIL(5)
      COMMON K15,K1,N,IELE,NE,NO
      COMMON /COESUB/A1,A2,A3,AIJK
      CALL DATE(IDATE)
      CALL TIME(ITIME)
      WRITE(6,90)IDATE,ITIME
      WRITE(6,100)
      READ(5,*)K1
      WRITE(6,105)
      READ(5,*)N
      IF(K1.EQ.1)WRITE(6,110)
      IF(K1.EQ.1)READ(5,120)(IELE(I),I=1,N)
      IF(K1.NE.1)WRITE(6,130)
      IF(K1.NE.1)READ(5,140)(IELE(I),NE(I),NO(I),I=1,N)
      WRITE(6,145)
      READ(5,*)K15
      WRITE(6,150)
      READ(5,160)KK1
      IF(KK1.EQ.'N ')GOTO 10
      WRITE(6,170)
      READ(6,180)NAMFIL
10    CALL ALPHA
      IF(KK1.EQ.'N ')GOTO 20
      CALL ASSIGN(3,NAMFIL,10)
      IF(K1.EQ.3)A1(1,3)=0.0
      IF(K1.EQ.3)WRITE(3,*,ERR=15)A1(1,3),(A1(I,2),I=1,N),(A1(I,1),
     + (A2(I,J),J=1,N),I=1,N)
      IF(K1.EQ.1)WRITE(3,*,ERR=15)((A1(I,J),J=1,N),(A2(I,J),J=1,N),
     + (A3(I,J),J=1,N),((AIJK(I,J,K),K=1,N),J=1,N),I=1,N)
      IF(K1.EQ.2)WRITE(3,*,ERR=15)((A1(I,J),J=1,N),(A2(I,J),J=1,N),
     + ((AIJK(I,J,K),K=1,N),J=1,N),I=1,N)
```

```
15      CALL CLOSE(3)
20      CALL DATE(IDATE)
        CALL TIME(ITIME)
        WRITE(6,95)IDATE,ITIME
        STOP
90      FORMAT(///1X,'DATE:  ',5A2,6X,'TIME:  ',4A2/)
95      FORMAT(1H1,//1X,'DATE:  ',5A2,6X,'TIME:  ',4A2/)
100     FORMAT(1X,'WHICH SYSTEM DO YOU WISH TO ANALYZE:'/3X,
     +  '1-ELEMENT SYSTEM  2-OXIDE SYSTEM  3-FUSED DISK SYSTEM  ?  ',$)
105     FORMAT(1X,'INPUT NUMBER OF ANALYTES:  ',$)
110     FORMAT(1X,'INPUT NAMES OF ANALYTES (XXS):  ',$)
120     FORMAT(12(A2,1X))
130     FORMAT(1X,'INPUT NAMES OF ANALYTES (XXNONS):  '/)
140     FORMAT(12(A2,I1,1X,I1,1X))
145     FORMAT(1X,'WHAT MASS ABS. COEF. ALGORITHM DO YOU WANT
     +TO USE :'/3X,'1-LEROUX ALGORITHM  2-HEINRICH ALGORITHM ?  ',$)
150     FORMAT(1X,'DO YOU WANT TO CREATE A DATAFILE FOR SAVING CALCULATE
     +D ALPHA COEFFICIENTS (Y/N)?  ',$)
160     FORMAT(A1)
170     FORMAT(1X,'INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX)
     +:  ',$)
180     FORMAT(5A2)
        END
```

```
      SUBROUTINE ALPHA
C
C       THIS SUBROUTINE CALCULATES ALPHA COEFFICIENTS FOR
C      INTERELEMENT EFFECT CORRECTION USED IN COLA EQUATION
C      FOR ELEMENT, OXIDE, OR FUSED DISK SYSTEMS.
C
C      NBS     04-SEP-1984
C
      REAL MAC,MU
      DIMENSION XINT(2,300),XINT1(2,11),IELE(12),NE(12),NO(12),
     + CL(12,4),ISR(12),IZ(12),A1(12,12),
     + A2(12,12),A3(12,12),AIJK(12,12,12),UCO(12),UC(12,12),C(5,3),
     + IE(12),G(5),ALFA(12),CAM(12),SWDB(12),SWDB1(12)
      COMMON K15,K1,N,IELE,NE,NO,KK2,CAM,IZ,ITP,ITS
      COMMON /TUBE1/XINT,XINT1,ND
      COMMON /TUBE2/IDTUBE,VOLT
      COMMON /BDSUB/TP,TS,C,CL,IE,UC,UCO,N5
      COMMON /COESUB/A1,A2,A3,AIJK
      DATA C/.001,.5,.999,.3,.3,.999,.5,.001,.7,.35,4*0.0,.35/
      IF(K1.NE.3)GOTO 4
      WRITE(6,950)
      DO 2 I=1,N
      WRITE(6,960)I,IELE(I),NE(I),NO(I)
      READ(5,*)CAM(I)
2     CONTINUE
      GOTO 5
4     IF(K1.EQ.1)GOTO 5
      C(1,1)=.2
      C(2,1)=.8
      C(1,2)=.8
      C(2,2)=.2
5     WRITE(6,1000)
      READ(5,*)ITP,ITS
      TP=1.0/SIN(FLOAT(ITP)*.0174533)
      TS=1.0/SIN(FLOAT(ITS)*.0174533)
      WRITE(6,1010)
      DO 10 I=1,N
      WRITE(6,1020)I,IELE(I)
      READ(5,*)ISR(I)
      CALL ATNUM(IELE(I),IZ(I))
      CALL CHAWV(CL(I,1),IELE(I),ISR(I))
      CALL ABSEDG(CL(I,2),IELE(I),ISR(I))
      CALL YIELD(Y,IELE(I),ISR(I))
      CALL JUMRAT(RJM,IELE(I),ISR(I))
      CL(I,3)=Y*RJM
      CL(I,4)=1.0
      IF(K1.NE.1)CALL AFIOX(CL(I,4),IELE(I),NE(I),NO(I))
      IE(I)=IELE(I)
10    CONTINUE
C
      WRITE(6,1022)
      READ(5,1024)KK2
      CALL TUBDAT
      IF(K1.EQ.3)CALL APAFD
      IF(K1.EQ.3) RETURN
      DO 170 II=1,N
      IF(K1.EQ.1.AND.KK2.EQ.'Y ')WRITE(6,1030)IDTUBE,VOLT,ITP,ITS,
     + IELE(II),IZ(II)
      IF(K1.EQ.2.AND.KK2.EQ.'Y ')WRITE(6,1040)IDTUBE,VOLT,ITP,ITS,
     + IELE(II),NE(II),NO(II),IZ(II)
      IF(KK2.EQ.'Y ')WRITE(6,1050)(IZ(I),I=1,N)
      IF(K1.EQ.1.AND.KK2.EQ.'Y ')WRITE(6,1060)(IELE(I),I=1,N)
      IF(K1.EQ.2.AND.KK2.EQ.'Y ')WRITE(6,1070)(IELE(I),NE(I),NO(I),
```

```
     +  I=1,N)
        DO 15 J=1,4
        Z=CL(1,J)
        CL(1,J)=CL(II,J)
        CL(II,J)=Z
15      CONTINUE
        NAM=IE(1)
        IE(1)=IE(II)
        IE(II)=NAM
        DO 20 I=1,N
        A1(II,I)=0.0
        A2(II,I)=0.0
        A3(II,I)=0.0
        DO 20 J=1,N
        AIJK(II,I,J)=0.0
20      CONTINUE
C
        ICAS=1
        N2=N
30      IF(ICAS.EQ.2)N2=N-1
        DO 110 M=2,N2
        DO 35 J=1,4
        Z=CL(2,J)
        CL(2,J)=CL(M,J)
        CL(M,J)=Z
35      CONTINUE
        NAM=IE(2)
        IE(2)=IE(M)
        IE(M)=NAM
        M1=M+1
        IF(ICAS.EQ.1)M1=N
        DO 100 MM=M1,N
        IF(ICAS.EQ.1)GOTO 40
        DO 38 J=1,4
        Z=CL(3,J)
        CL(3,J)=CL(MM,J)
        CL(MM,J)=Z
38      CONTINUE
        NAM=IE(3)
        IE(3)=IE(MM)
        IE(MM)=NAM
40      CONTINUE
C
        IF(ICAS.EQ.1)N5=2
        IF(ICAS.EQ.2)N5=3
        DO 50 J=1,N5
        IF(K15.EQ.1)UCO(J)=MU('O ',CL(J,1))
        IF(K15.EQ.2)UCO(J)=MAC('O ',CL(J,1))
        DO 50 K=1,N5
        IF(K15.EQ.1)UC(J,K)=MU(IE(J),CL(K,1))
        IF(K15.EQ.2)UC(J,K)=MAC(IE(J),CL(K,1))
50      CONTINUE
        I1=1
        I2=4
        IF(ICAS.EQ.2)I1=5
        IF(ICAS.EQ.2)I2=5
        DO 90 I=I1,I2
        SW1=0.0
        SWDB1(1)=0.0
        KK5=1
        IF(IDTUBE.EQ.'CR'.AND.IE(1).EQ.'CR')KK5=2
        IF(IDTUBE.EQ.'CR'.AND.IE(1).EQ.'MN')KK5=2
        K12=0
        DO 60 K=1,ND
```

```
      IF(XINT(1,K).GT.CL(1,2))GOTO 70
      CALL BDCOEF(SW,SWDB,SWLOI,I,XINT(1,K),XINT(2,K),K1,KK5,K15,K12)
      SW1=SW1+SW
      SWDB1(1)=SWDB1(1)+SWDB(1)
60    CONTINUE
70    DO 80 K=1,11
      IF(XINT1(1,K).EQ.0.0)GOTO 80
      IF(XINT1(1,K).GT.CL(1,2))GOTO 80
      CALL BDCOEF(SW,SWDB,SWLOI,I,XINT1(1,K),XINT1(2,K),K1,KK5,
     +            K15,K12)
      SW1=SW1+SW
      SWDB1(1)=SWDB1(1)+SWDB(1)
80    CONTINUE
C
      G(I)=(SW1/SWDB1(1)-1.0)/C(I,2)
90    CONTINUE
C
      IF(ICAS.EQ.1)GOTO 100
      AIJK(II,MM,M)=(G(5)*C(5,2)-ALFA(M)*C(5,2)-ALFA(MM)*C(5,3))
     + /(C(5,2)*C(5,3))
      DO 95 J=1,4
      Z=CL(MM,J)
      CL(MM,J)=CL(3,J)
      CL(3,J)=Z
95    CONTINUE
      NAM=IE(MM)
      IE(MM)=IE(3)
      IE(3)=NAM
100   CONTINUE
C
      IF(ICAS.EQ.2)GOTO 110
      IF(K1.EQ.1)A1(II,M)=G(3)
      IF(K1.EQ.2)A1(II,M)=(G(1)*C(2,2)-G(2)*C(1,2))/(C(2,2)-
     + C(1,2))
      IF(K1.EQ.1)A2(II,M)=G(1)-G(3)
      IF(K1.EQ.2)A2(II,M)=(G(2)-G(1))/(C(2,2)-C(1,2))
      IF(K1.EQ.1)A3(II,M)=(G(1)-G(2))/(G(2)-G(3))-1.0
      IF(K1.EQ.2)A3(II,M)=0.0
      ALFA(M)=G(4)
110   CONTINUE
      IF(ICAS.EQ.2)GOTO 120
      IF(N.EQ.2)GOTO 120
      DO 118 I=3,N
      I1=I-1
      DO 115 J=1,4
      Z=CL(I1,J)
      CL(I1,J)=CL(I,J)
      CL(I,J)=Z
115   CONTINUE
      NAM=IE(I1)
      IE(I1)=IE(I)
      IE(I)=NAM
118   CONTINUE
      ICAS=ICAS+1
      GOTO 30
C
120   IF(II.EQ.1)GOTO 150
      DO 140 J=2,II
      JJ=J-1
      Z=A1(II,JJ)
      A1(II,JJ)=A1(II,J)
      A1(II,J)=Z
      Z=A2(II,JJ)
      A2(II,JJ)=A2(II,J)
```

```
      A2(II,J)=Z
      Z=A3(II,JJ)
      A3(II,JJ)=A3(II,J)
      A3(II,J)=Z
      DO 130 I=2,II
      I1=I-1
      Z=AIJK(II,I1,J)
      AIJK(II,I1,J)=AIJK(II,I,J)
      AIJK(II,I,J)=Z
130   CONTINUE
      DO 140 I=2,N
      Z=AIJK(II,I,JJ)
      AIJK(II,I,JJ)=AIJK(II,I,J)
      AIJK(II,I,J)=Z
140   CONTINUE
150   CONTINUE
C
      IF(KK2.EQ.'N ')GOTO 170
      WRITE(6,1080)(A1(II,J),J=1,N)
      WRITE(6,1090)(A2(II,J),J=1,N)
      IF(K1.EQ.1)WRITE(6,1100)(A3(II,J),J=1,N)
      IF(K1.EQ.1)WRITE(6,1110)IZ(1),IELE(1),AIJK(II,1,1)
      IF(K1.EQ.2)WRITE(6,1120)IZ(1),IELE(1),NE(1),NO(1),AIJK(II,1,1)
      DO 160 J=2,N
      NA=J-1
      IF(K1.EQ.1)WRITE(6,1130)IZ(J),IELE(J),(AIJK(II,J,K),K=1,NA)
      IF(K1.EQ.2)WRITE(6,1140)IZ(J),IELE(J),NE(J),NO(J),
     +  (AIJK(II,J,K),K=1,NA)
160   CONTINUE
C
      N2=N-1
      IF(N2.LT.3)GOTO 170
      DO 168 I=3,N2
      I1=I-1
      DO 165 J=1,4
      Z=CL(I1,J)
      CL(I1,J)=CL(I,J)
      CL(I,J)=Z
165   CONTINUE
      NAM=IE(I1)
      IE(I1)=IE(I)
      IE(I)=NAM
168   CONTINUE
170   CONTINUE
190   RETURN
950   FORMAT(1X,'INPUT MEAN CONCENTRATIONS (WEIGHT FRACTION) OF ANALYT
     +ES IN THE SPECIMENS TO BE ANALYZED:')
960   FORMAT(3X,'I=',I2,4X,A2,I1,1HO,I1,4X,$)
1000  FORMAT(1X,'FOR SAMPLE GEOMETRY, INPUT INCIDENCE & EMERGENCE ANGL
     +ES (DEGREE-XX):  ',$)
1010  FORMAT(1X,'INPUT THE CHARACTERISTIC LINE NUMBER YOU WISH TO MEAS
     +URE (1-KA, 2-KB, 3-LA1, 4-LB1, 5-LB2):')
1020  FORMAT(1X,'I=',I2,4X,A2,4X,$)
1022  FORMAT(1X,'DO YOU WANT TO PRINT OUT CALCULATED ALPHA COEFFICIENT
     +S(Y/N):  ',$)
1024  FORMAT(A1)
1030  FORMAT(1H1,//,41X,'BASIC ALPHA COEFFICIENTS FOR USE IN COLA
     +EQUATION'//58X,'(ELEMENTAL SYSTEM)',////,
     +  55X,'  TARGET: ',A2,2X,F5.1,' KV',/,
     +  55X,'GEOMETRY: ',I2,',',I2,' DEGREES',///,
     +  58X,' ANALYTE: ',A2,1X,'(',I2,')',//)
1040  FORMAT(1H1,//,41X,'HYBRID ALPHA COEFFICIENTS FOR USE IN COLA
     + EQUATION'//58X,'(OXIDE    SYSTEM)',////,
     +  55X,'  TARGET: ',A2,2X,F5.1,' KV',/,
```

```
     +  55X,'GEOMETRY: ',I2,',',I2,' DEGREES',///,
     +  56X,' ANALYTE: ',A2,I1,'O',I1,1X,'(',I2,')',//)
1050    FORMAT(16X,16(5X,I2,1X),/)
1060    FORMAT(/17X,16(4X,A2,2X),/)
1070    FORMAT(/18X,16(2X,A2,I1,'O',I1,1X),/)
1080    FORMAT(/11X,'A1',4X,12F8.3)
1090    FORMAT(/11X,'A2',4X,12F8.3)
1100    FORMAT(/11X,'A3',4X,12F8.3)
1110    FORMAT(/5X,'AIJK  ',I2,1X,A2,1X,F8.3,1X)
1120    FORMAT(/2X,'AIJK  ',I2,1X,A2,I1,'O',I1,1X,F8.3,1X)
1130    FORMAT(/11X,I2,1X,A2,1X,12F8.3)
1140    FORMAT(/8X,I2,1X,A2,I1,'O',I1,1X,12F8.3)
        END
```

```
      SUBROUTINE APAFD
C
C       THIS SUBROUTINE PERFORMS MOST OF THE CALCULATION FOR
C      OBTAINING THE ALPHA COEFFICIENTS USED IN FUSED DISC
C      SYSTEM.
C
C      NBS     04-SEP-84
C
      REAL MAC,MU
      DIMENSION CAM(12),UCO(12),UCF(12),SWDB1(12),XINT(2,300),
     +          XINT1(2,11),UC(12,12),IELE(12),NE(12),NO(12),
     +          C(5,3),CL(12,4),IE(12),A1(12,12),A2(12,12)
      DIMENSION SWDB(12),IZ(12)
      COMMON K15,K1,N,IELE,NE,NO,KK2,CAM,IZ,ITP,ITS
      COMMON /COESUB/A1,A2
      COMMON /TUBE1/XINT,XINT1,ND
      COMMON /TUBE2/IDTUBE,VOLT
      COMMON /BDSUB/TP,TS,C,CL,IE,UC,UCO,N5,UCF,CA,CB,F,CLOI
      COMMON /WFRA/WLI,WB,WO,WF
      DATA CLOI/.25/
      N5=N
      WRITE(6,190)
      READ(5,*)K12
      GL=0.
      WRITE(6,180)
  180 FORMAT(' GRAMS OF SAMPLE:',$)
      READ(5,*)GS
      WRITE(6,182)
  182 FORMAT(' GRAMS OF LI2B407:',$)
      READ(5,*)GF
      IF(K12.EQ.1) GO TO 4
      IF(K12.EQ.2) WRITE(6,184)
  184 FORMAT(' GRAMS OF LIF:',$)
      IF(K12.EQ.3) WRITE(6,186)
  186 FORMAT(' GRAMS OF LIBO2:',$)
      READ(5,*)GL
    4 CONTINUE
      TWT=GF+GL
      F=GS/(TWT+GS)
      GO TO (6,7,8),K12
    6 WLI=.0821
      WB=.2557
      WF=0.
      WO=.6623
      GO TO 9
    7 WLI=(GF*.0821+GL*.2675)/TWT
      WB=GF*.2557/TWT
      WO=GF*.6623/TWT
      WF=GL*.7325/TWT
      GO TO 9
    8 WLI=(GF*.0821+GL*.1395)/TWT
      WB=(GF*.2557+GL*.2173)/TWT
      WO=(GF*.6623+GL*.6432)/TWT
      WF=0.
    9 CONTINUE
      IF(KK2.NE.'Y ')GOTO 5
      WRITE(6,192)IDTUBE,VOLT,ITP,ITS,(IZ(I),I=1,N)
      WRITE(6,194)(IELE(I),NE(I),NO(I),I=1,N)
      WRITE(6,196)(CAM(I),I=1,N)
      WRITE(6,198)
5     DO 100 I=1,N
```

```
      CA=CAM(I)
      CB=1.0-CA
      DO 10 J=1,4
      Z=CL(1,J)
      CL(1,J)=CL(I,J)
      CL(I,J)=Z
10    CONTINUE
      NAM=IE(1)
      IE(1)=IE(I)
      IE(I)=NAM
C
      DO 20 J=1,N
      IF(K15.EQ.2) GO TO 15
C  K15 EQUALS 1
      UCO(J)=MU('O ',CL(J,1))
      UCF(J)=WLI*MU('LI',CL(J,1))+WB*
     1 MU('B ',CL(J,1))+WO*UCO(J)+WF*MU('F ',CL(J,1))
      GO TO 18
C  K15 EQUALS 2
   15 UCO(J)=MAC('O ',CL(J,1))
      UCF(J)=WLI*MAC('LI',CL(J,1))+WB*
     1 MAC('B ',CL(J,1))+WO*UCO(J)+WF*MAC('F ',CL(J,1))
   18 CONTINUE
      SWDB1(J)=0.0
      DO 20 K=1,N
      IF(K15.EQ.1)UC(J,K)=MU(IE(J),CL(K,1))
      IF(K15.EQ.2)UC(J,K)=MAC(IE(J),CL(K,1))
20    CONTINUE
      SW1=0.0
      SWLOI1=0.0
      KK5=1
      IF(IDTUBE.EQ.'CR'.AND.IE(1).EQ.'CR')KK5=2
      IF(IDTUBE.EQ.'CR'.AND.IE(1).EQ.'MN')KK5=2
      DO 40 K=1,ND
      IF(XINT(1,K).GT.CL(1,2))GOTO 50
      CALL BDCOEF(SW,SWDB,SWLOI,1,XINT(1,K),XINT(2,K),K1,KK5,K15,K12)
      SW1=SW1+SW
      SWLOI1=SWLOI1+SWLOI
      DO 30 J=2,N
      SWDB1(J)=SWDB1(J)+SWDB(J)
30    CONTINUE
40    CONTINUE
50    DO 70 K=1,11
      IF(XINT1(1,K).EQ.0.0)GOTO 70
      IF(XINT1(1,K).GT.CL(1,2))GOTO 70
      CALL BDCOEF(SW,SWDB,SWLOI,1,XINT1(1,K),XINT1(2,K),K1,KK5,
     +            K15,K12)
      SW1=SW1+SW
      SWLOI1=SWLOI1+SWLOI
      DO 60 J=2,N
      SWDB1(J)=SWDB1(J)+SWDB(J)
60    CONTINUE
70    CONTINUE
C
      A2(I,1)=0.0
      DO 80 J=2,N
      RA=CA*SWDB1(J)/SW1
      A2(I,J)=(CA/RA-1.0)/CB
80    CONTINUE
      A1(I,1)=(SW1*(1.0-F*CLOI)/SWLOI1-1.0)/CLOI
      A1(I,2)=0.0
C
```

```
      IF(I.EQ.1)GOTO 100
      DO 90 J=2,I
      JJ=J-1
      Z=A2(I,JJ)
      A2(I,JJ)=A2(I,J)
      A2(I,J)=Z
90    CONTINUE
100   CONTINUE
C
      IF(KK2.NE.'Y ')RETURN
      DO 110 I=1,N
      WRITE(6,200)IZ(I),IELE(I),NE(I),NO(I),A1(I,1),(A2(I,J),J=1,N)
110   CONTINUE
      IF(K12.EQ.1)WRITE(6,210)GS,GF
      IF(K12.EQ.2)WRITE(6,220)GS,GF,GL
      IF(K12.EQ.3)WRITE(6,230)GS,GF,GL
      RETURN
190   FORMAT(1X,'WHAT FLUX CONDITIONS DO YOU WISH :'/
     +  3X,'1-SAMPLE + LI2B4O7',/
     +  3X,'2-SAMPLE + LI2B4O7 + LIF',/
     +  3X,'3-SAMPLE + LI2B4O7 + LIBO2 ?  ',$)
192   FORMAT(1H1,//36X,'MODIFIED ALPHA COEFFICIENTS FOR USE IN COLA EQ
     +UATION'//57X,'(FUSED DISK SYSTEM)',////,
     +  55X,'  TARGET: ',A2,2X,F5.1,' KV',/
     +  55X,'GEOMETRY: ',I2,',',I2,'  DEGREES',///,
     +  58X,'MATRIX CONSTITUENTS'//18X,12(6X,I2))
194   FORMAT(/15X,'LOI',3X,12(1X,A2,I1,1HO,I1,2X))
196   FORMAT(/1X,'MEAN CONC.',2X,' 25.00  ',12(2PF6.2,2X))
198   FORMAT(/3X,'ANALYTE')
200   FORMAT(/2X,I2,2X,A2,I1,1HO,I1,13F8.3)
210    FORMAT(///1X,'* FUSED DISK :',F6.4,'G SAMPLE +',F6.4,'G LI2B4O7')
220    FORMAT(///' * FUSED DISK :',F6.4,'G SAMPLE +',F6.4,'G LI2B4O7 +',
     +F6.4,'G LIF')
230    FORMAT(///1X,'* FUSED DISK :',F6.4,'G SAMPLE +',F6.4,'G LI2B4O7',
     +F6.4,'LIBO2')
      END
```

```
      SUBROUTINE ATNUM(INAM,IZ)
C
C     THIS SUBROUTINE PROVIDES THE ATOMIC NUMBER WHEN A
C     CORRESPONDING ELEMENT NAME IS GIVEN.
C
C     NBS      04-SEP-1984
C
      DIMENSION ID(94)
      DATA ID/'H ','HE','LI','BE','B ','C ','N ','O ','F ',
     1 'NE','NA','MG','AL','SI','P ','S ','CL','AR','K ','CA',
     1 'SC','TI','V ','CR','MN','FE','CO','NI','CU','ZN','GA',
     1 'GE','AS','SE','BR','KR','RB','SR','Y ',
     1 'ZR','NB','MO','TC','RU','RH','PD','AG','CD','IN','SN',
     1 'SB','TE','I ','XE','CS','BA','LA','CE','PR','ND','PM',
     1 'SM','EU','GD','TB','DY','HO','ER','TM','YB','LU','HF',
     1 'TA','W ','RE','OS','IR','PT','AU','HG','TL','PB','BI',
     1 'PO','AT','RN','FR','RA','AC','TH','PA','U ','NP','PU'/
      DO 10 I=1,94
       IF(INAM.EQ.ID(I)) GO TO 20
10    CONTINUE
      WRITE(6,100)INAM
      STOP
20    IZ=I
100   FORMAT(/1X,'ERROR: ',A2,' IS NOT A CORRECT ELEMENT NAME AMONG 1
     +H-94 PU.')
      RETURN
      END


      SUBROUTINE CHAWV(WV,IELE,ISR)
C
C     THIS SUBROUTINE PROVIDES CHARACTERISTIC LINE
C     WAVELENGTHS (KA,KB,LA1,LB1,LB2) BY MEANS OF AN
C     EMPIRICAL FIT. THIS FIT IS NOT RECOMMENDED FOR
C     LINES BELOW 1 KEV.
C
C     NBS      04-SEP-1984
C
      DIMENSION D1(5),D2(5),D3(5)
      DATA D1/-.0199726,-.060101,-.123941,-.00322523,-.197431/
      DATA D2/2.22412,2.52781,3.29533,2.48613,4.01718/
      DATA D3/-5.1774,-5.6437,-9.75836,-8.37742,-11.3323/
      CALL ATNUM(IELE,IZ)
      ZI=IZ
      ZL=ALOG(ZI)
      WV=12.398/EXP(D1(ISR)*ZL*ZL+D2(ISR)*ZL+D3(ISR))
      RETURN
      END
```

```
      SUBROUTINE ABSEDG(WV,IELE,ISR)
C
C     THIS SUBROUTINE CALCULATES THE WAVELENGTH OF AN ABSORPTION
C     EDGE FROM THE CHARACTERISTIC LINE WAVELENGTH.
C     THIS EMPIRICAL FIT IS NOT RECOMMENDED BELOW 1 KEV.
C
C     NBS     04-SEP-1984
C
      DIMENSION C1(3),C2(3),C3(3)
      DATA C1/-.0397931,-.0865397,-.2283427/
      DATA C2/2.423000,3.323153,4.311724/
      DATA C3/5.509104,10.25054,12.00253/
      CALL ATNUM(IELE,IZ)
      ZI=IZ
      ZL=ALOG(ZI)
      IF(ISR.EQ.1.OR.ISR.EQ.2)WV=EXP(C1(1)*ZL*ZL+C2(1)*ZL-C3(1))
      IF(ISR.EQ.3.OR.ISR.EQ.5)WV=EXP(C1(3)*ZL*ZL+C2(3)*ZL-C3(3))
      IF(ISR.EQ.4)WV=EXP(C1(2)*ZL*ZL+C2(2)*ZL-C3(2))
      WV=12.398/WV
      RETURN
      END


      SUBROUTINE JUMRAT(JUMP,IELE,ISR)
C
C     THIS SUBROUTINE PROVIDES JUMP RATIOS (1-1/R)
C     FOR K OR L III ABSORPTION EDGES.
C     FROM REFERENCE: E.P.BERTIN, 'PRINCIPLES & PRACTICE OF
C                     X-RAY SPECTROMETRIC ANALYSIS' SECOND
C                     EDITION, 1975. P977-979
C
C     NBS     04-SEP-1984
C
      DIMENSION JK(94),JL(94)
      REAL JK,JL,JUMP
      DATA JK/3*1.0,.970,.965,.959,.953,.948,.943,.937,.932,.927,
     +        .921,.916,.911,.903,.895,.899,.887,.890,.883,.883,.886,
     +        .886,.884,.878,.881,.873,.874,.868,.865,.862,.861,.855,
     +        .857,.858,.854,.858,.854,.852,.860,.856,.853,.852,.847,
     +        .856,.848,.846,.840,.845,.843,.839,.838,.835,.832,.828,
     +        .835,.830,.828,.833,.831,.827,.824,.827,.819,.818,.812,
     +        .818,.813,.807,.808,.816,.801,.805,.791,.803,.807,.805,
     +        .797,.801,.795,.791,.788,2*0.0,.788,3*0.0,.772,0.0,
     +        .773,0.0,.779/
      DATA JL/27*0.0,.639,.652,.824,.824,.825,.795,.782,.782,.760,
     +        .763,.744,.752,.748,.735,.728,.722,.708,.731,.706,
     +        .690,.692,.693,.673,.660,.664,.650,.653,.649,.648,
     +        .632,.635,.629,.624,.630,.627,.633,.630,.631,.636,.650,
     +        .659,.637,.611,.618,.586,.615,.618,.626,.605,.581,
     +        .620,.590,.583,.600,.591,.572,2*0.0,.573,3*0.0,.581,
     +        0.0,.562,0.0,.556/
      CALL ATNUM(IELE,IZ)
      IF(ISR.EQ.1.OR.ISR.EQ.2)JUMP=JK(IZ)
      IF(ISR.EQ.3.OR.ISR.EQ.4.OR.ISR.EQ.5)JUMP=JL(IZ)
      RETURN
      END
```

```
      SUBROUTINE YIELD(Y,IELE,ISR)
C
C     THE SUBROUTINE PROVIDES X-RAY FLUORESCENT YIELDS FOR K,
C     L II OR L III SERIES LINES BY MEANS OF EMPIRICAL FITS.
C
C     NBS     04-SEP-1984
C
      CALL ATNUM(IELE,IZ)
      ZI=IZ
      ZL=ALOG(ZI)
      IF(ISR.EQ.3.OR.ISR.EQ.5)GOTO 10
      IF(ISR.EQ.4)GOTO 20
      OM1=(.015+.0327*ZI-6.4E-7*ZI**3)**4
      Y=OM1/(1.0+OM1)
      RETURN
10    OM1=(-.901+.0466*ZI-4.961E-4*ZI*ZI+2.296E-6*ZI**3)**4
      Y=OM1/(1.0+OM1)
      RETURN
20    OM1=(.491-.010*ZI+2.55E-4*ZI*ZI-9.20E-7*ZI**3)**4
      Y=OM1/(1.0+OM1)
      RETURN
      END



      SUBROUTINE AFIOX(AFOX,IELE,NE,NO)
C
C     THIS SUBROUTINE CALCULATES THE ATOMIC FRACTION OF THE
C     ANALYTE IN A DEFINED OXIDE.
C
C     NBS     04-SEP-1984
C
      CALL SBATWT('O ',AWO)
      CALL SBATWT(IELE,AWE)
      AFOX=AWE*FLOAT(NE)
      AFOX=AFOX/(AFOX+AWO*FLOAT(NO))
      RETURN
      END
```

```
      SUBROUTINE BDCOEF(SW,SWDB,SWLOI,I,WV1,WV2,K1,KK5,K15,K12)
C
C       THIS SUBROUTINE CALCULATES BETA AND DELTA COEFFICIENTS
C       IN MODIFIED VERSION OF SHERMAN'S EQUATION AT A CERTAIN
C       WAVELENGTH AND CORRESPONDING X-RAY TUBE SPECTRAL INTENSITY.
C
C       NBS     31-OCT-1984
C
      REAL MAC,MU
      DIMENSION C(5,3),CL(12,4),U(12),BETA(12),DELTA(12),UC(12,12),
     +          IE(12),UCO(12),UCF(12),SWDB(12)
      COMMON /BDSUB/TP,TS,C,CL,IE,UC,UCO,N5,UCF,CA,CB,F,CLOI
      COMMON/WFRA/WLI,WB,WO,WF
      IF(K15.EQ.2) GO TO 4
C  K15 EQUALS 1
      UO=MU('O ',WV1)
      UF=WLI*MU('LI',WI1)+WB*MU('B ',WV1)+ WO*UO+WF*MU(' ',WV1)
      GO TO 6
   4  CONTINUE
C  K15 EQUALS 2
      UO=MAC('O ',WV1)
      UF=WLI*MAC('LI',WV1)+WB*MAC('B ',WV1)+WO*UO+WF*MAC('F ',WV1)
   6  CONTINUE
      DO 10 J=1,N5
      IF(K15.EQ.1)U(J)=MU(IE(J),WV1)
      IF(K15.EQ.2)U(J)=MAC(IE(J),WV1)
10    CONTINUE
C
C     CALCULATION OF BETA COEFFICIENTS
C     0.081 G/CM2 AL FILTER IS USED FOR ANALYTES CR & MN
C     WHEN CR TARGET OF X-RAY TUBE IS EMPLOYED.
C
      IF(KK5.EQ.2.AND.K15.EQ.1)WV2=WV2*EXP(-.081*MU('AL',WV1))
      IF(KK5.EQ.2.AND.K15.EQ.2)WV2=WV2*EXP(-.081*MAC('AL',WV1))
      DEN=CL(1,4)*(U(1)*TP+UC(1,1)*TS)+(1.0-CL(1,4))*(UO*TP+UCO(1)*TS)
      W=U(1)*WV2/DEN
      IF(KK5.EQ.2.AND.K15.EQ.1)WV2=WV2/EXP(-.081*MU('AL',WV1))
      IF(KK5.EQ.2.AND.K15.EQ.2)WV2=WV2/EXP(-.081*MAC('AL',WV1))
      IF(K1.EQ.3)PHIF=(UF*TP+UCF(1)*TS)/DEN-1.0
      IF(K1.NE.3)SBETA=0.0
      N2=2
      IF(K1.EQ.3)N2=1
      DO 20 J=N2,N5
      BETA(J)=(CL(J,4)*(U(J)*TP+UC(J,1)*TS)+(1.0-CL(J,4))*(UO*TP+
     +  UCO(1)*TS))/DEN-1.0
      IF(K1.NE.3)SBETA=SBETA+C(I,J)*BETA(J)
20    CONTINUE
C
C     CALCULATION OF DELTA COEFFICIENTS
C
      IF(K1.NE.3)SDELTA=0.0
      DO 60 J=1,N5
      IF(WV1.GT.CL(J,2).OR.CL(J,1).GT.CL(1,2))GOTO 40
      IF(K1.EQ.3)GOTO 32
      UE=0.0
      UEI=0.0
      UEJ=0.0
      DO 30 L=1,N5
      UE=UE+(CL(L,4)*U(L)+(1.0-CL(L,4))*UO)*C(I,L)*TP
      UEI=UEI+(CL(L,4)*UC(L,1)+(1.0-CL(L,4))*UCO(1))*C(I,L)*TS
      UEJ=UEJ+(CL(L,4)*UC(L,J)+(1.0-CL(L,4))*UCO(J))*C(I,L)
```

```
30      CONTINUE
        GOTO 34
32      UE=((CL(1,4)*U(1)+(1.0-CL(1,4))*UO)*CA+(CL(J,4)*U(J)+(1.0-
     +  CL(J,4))*UO)*CB)*TP
        UE=F*UE+(1.0-F)*UF*TP
        UEI=((CL(1,4)*UC(1,1)+(1.0-CL(1,4))*UCO(1))*CA+(CL(J,4)*
     +  UC(J,1)+(1.0-CL(J,4))*UCO(1))*CB)*TS
        UEI=F*UEI+(1.0-F)*UCF(1)*TS
        UEJ=(CL(1,4)*UC(1,J)+(1.0-CL(1,4))*UCO(J))*CA+(CL(J,4)*
     +  UC(J,J)+(1.0-CL(J,4))*UCO(J))*CB
        UEJ=F*UEJ+(1.0-F)*UCF(J)
34      T1=.5*CL(J,3)*CL(J,4)*UC(1,J)*U(J)/U(1)
        T2=(ALOG(1.0+UE/UEJ))/UE
        T3=(ALOG(1.0+UEI/UEJ))/UEI
        DELTA(J)=T1*(T2+T3)
        GOTO 50
40      DELTA(J)=0.0
50      IF(K1.NE.3)SDELTA=SDELTA+C(I,J)*DELTA(J)
60      CONTINUE
        IF(K1.EQ.3)GOTO 70
        SW=W
        SWDB(1)=W*(1.0+SDELTA)/(1.0+SBETA)
        RETURN
70      SW=W/(1.0+(1.0-F)*PHIF)
        CF=(1.0-F)/(1.0-F*CLOI)
        SWLOI=W/(1.0+CF*PHIF)
        DO 80 J=2,N5
        SWDB(J)=W*(1.0+F*CB*DELTA(J))/(1.0+F*CB*BETA(J)+(1.0-F)*PHIF)
80      CONTINUE
        RETURN
        END
```

```
      SUBROUTINE TUBDAT
C
C       THIS SUBROUTINE PROVIDES THE X-RAY TUBE SPECTRAL DISTRIBUTION
C      NEEDED FOR CALCULATING ALPHA COEFFICIENTS BY USING EITHER THE
C      NBS ALGORITHM OR MEASURED DATA FROM THE LITERATURE.
C
C      NBS     04-SEP-1984
C
      DIMENSION XINT(2,300),IDLINE(4),DATTGT(2,11),DFSP(6),
     +  XINT1(2,11)
      COMMON K15
      COMMON /TUBE1/XINT,XINT1,ND
      COMMON /TUBE2/IDTUBE,VOLT,TOFAGL,WINTHI
      DATA IDLINE/'KA','KB','LA','LB'/
      WRITE(6,100)
      READ(5,*)K11
      WRITE(6,105)
      READ(5,125)KK11
      WRITE(6,140)
      READ(5,125)IDTUBE
      WRITE(6,150)
      READ(5,*)VOLT,TOFAGL,WINTHI
      IF(K11.EQ.1)GOTO 10
      WRITE(6,110)
      READ(5,120)DFSP
      WRITE(6,130)
      READ(5,*)ND
      OPEN(UNIT=3,NAME=DFSP,TYPE='OLD')
      READ(3,*,ERR=5)((XINT(I,J),J=1,ND),I=1,2),((XINT1(I,J),J=1,11),
     +  I=1,2)
5     CLOSE(UNIT=3)
      GOTO 50
10    WRITE(6,160)
      READ(5,*)EDGE
      WVMIN=12.398/VOLT
      ND=IFIX((EDGE-WVMIN)/.02)+1
      WV=WVMIN
      XINT(1,1)=WVMIN
      XINT(2,1)=0.0
      DO 20 I=2,ND
      WV=WV+.02
      XINT(1,I)=WV
      CALL CTNLIN(XINT(2,I),WV)
20    CONTINUE
      CALL INFTGT(K12,IDLINE,DATTGT,IDTUBE)
      DO 25 I=1,11
      XINT1(1,I)=0.0
      XINT1(2,I)=0.0
25    CONTINUE
      DO 30 I=1,4
      IF(IDLINE(I).EQ.'  ')GOTO 30
      XINT1(1,I)=DATTGT(1,I)
      CALL CHALIN(CINT,DATTGT(1,I),IDLINE(I))
      IF(IDLINE(I).EQ.'LA')RLA=CINT
      XINT1(2,I)=CINT*50.0
30    CONTINUE
      IF(K12.EQ.1)GOTO 50
      DO 40 I=5,11
      IF(K12.EQ.2.AND.I.GT.8)GOTO 50
      XINT1(1,I)=DATTGT(1,I)
      CINT=RLA*DATTGT(2,I)
      XINT1(2,I)=CINT*50.0
40    CONTINUE
```

```
50      IF(KK11.EQ.'N ')GOTO 60
        IF(K11.EQ.1)WRITE(6,180)
        IF(K11.EQ.2)WRITE(6,190)
        WRITE(6,200)IDTUBE,VOLT,TOFAGL,WINTHI,(XINT(1,I),XINT(2,I)
     +  ,I=1,ND)
        WRITE(6,210)((XINT1(I,J),J=1,11),I=1,2)
        WRITE(6,220)
60      RETURN
100     FORMAT(' WHICH X-RAY TUBE SPECTRAL DISTRIBUTION DO YOU PREFER:'
     +  /3X,'1-CALCULATED SPECTRUM FROM NBS ALGORITHM  ;  2-MEASURED SPE
     +CTRUM ?  ',$)
105     FORMAT(1X,'DO YOU WANT TO PRINT OUT THE SPECTRAL DISTRIBUTION(Y/
     +N) ?  ',$)
110     FORMAT(' INPUT THE DATAFILE NAME OF X-RAY TUBE SPECTRUM(XXXXXX.X
     +XX) :  ',$)
120     FORMAT(6A4)
125     FORMAT(A2)
130     FORMAT(1X,'INPUT TOTAL NUMBER OF WAVELENGTH INTERVALS FOR CONTIN
     +UUM (MAX.=300) :  ',$)
140     FORMAT(1X,'INPUT NAME OF X-RAY TUBE TARGET (XX) :  ',$)
150     FORMAT(' INPUT VOLTAGE(KV), TAKE-OFF ANGLE OF X-RAY FROM TUBE TA
     +RGET(DEGREE), AND'/'    WINDOW THICKNESS(MM) OF X-RAY TUBE :  ',$)
160     FORMAT(1X,'INPUT THE ENDING WAVELENGTH OF X-RAY TUBE SPECTRUM(AN
     +GSTROM) :  ',$)
180     FORMAT(1H1,////36X,'CALCULATED X-RAY TUBE SPECTRAL DISTRIBUTION
     +  ',/47X,'USING NBS ALGORITHM')
190     FORMAT(1H1,////,37X,'MEASURED X-RAY TUBE SPECTRAL DISTRIBUTION
     +  ')
200     FORMAT(//34X,'X-RAY TUBE TARGET: ',A2,4X,'KV: ',F5.1,4X,/,
     +  27X,'TAKE-OFF ANGLE(DEGREE): ',F4.1,4X,'BE WINDOW THICKNESS(MM):
     + ',F5.3,///,3X,'LAMDA(A)',5X,'I*.02A',4X,'LAMDA(A)',5X,
     +  'I*.02A',4X,'LAMDA(A)',5X,,'I*.02A',4X,'LAMDA(A)',5X,'I*.02A',
     +  4X,'LAMDA(A)',5X,'I*.02A',//(1X,5(F9.4,2X,E12.4)))
210     FORMAT(///6X,'KA',10X,'KB',10X,'LA1',9X,'LB1',9X,'LB2',
     +  9X,'LB3',9X,'LB4',9X,'LG1',9X,'LG2',9X,'LG3',9X,'LL',//
     +  11(F10.4,2X)/11E12.4)
220     FORMAT(///)
        END
```

```
      SUBROUTINE CTNLIN(HINT,WV)
C
C     THIS SUBROUTINE CALCULATES THE CONTINUUM INTENSITY OF THE X-RAY
C     TUBE SPECTRUM AT A GIVEN WAVELENGTH USING THE NBS ALGORITHM.
C     (UNIT: PHOTONS/A/E/STRD)
C
C     NBS     04-SEP-1984
C
      REAL MAC,MU
      COMMON K15
      COMMON /TUBE2/IDTUBE,VOLT,TOFAGL,WINTHI
      WVMIN=12.398/VOLT
      TB=.185*WINTHI
      R=.0174533*TOFAGL
      CALL ATNUM(IDTUBE,IZ)
      Z=FLOAT(IZ)
      IF(K15.EQ.1)PSE=MU(IDTUBE,WV)*(WVMIN**(-1.65)-WV**(-1.65))/
     +  SIN(R)
      IF(K15.EQ.2)PSE=MAC(IDTUBE,WV)*(WVMIN**(-1.65)-WV**(-1.65))/
     +  SIN(R)
      F=1.0+PSE*(1.0+(1.0+2.56E-3*Z**2)**(-1))/(1.0+2.56E3*WVMIN
     +  *Z**(-2))/(.25*PSE+1.0E4)
      HINT=2.72E-6*Z*(WV/WVMIN-1.0)*WV**(-2)*F**(-2)*
     +  EXP(-.35*TB*WV**2.86)
      RETURN
      END


      SUBROUTINE INFTGT(K1,IDLINE,DATTGT,IDTUBE)
C
C     THE SUBROUTINE PROVIDES THE DATA NEEDED
C     FOR CALCULATING CHARACTERISTIC LINE INTENSITY
C     OF AN X-RAY TUBE SPECTRUM.
C
C     NBS     04-SEP-1984
C
      DIMENSION IDLINE(4),IDTGT(7),DATTGT(2,11)
      DATA IDTGT/'SC','CR','MO','RH','AG','W ','AU'/
      K1=2
      IF(IDTUBE.EQ.'SC'.OR.IDTUBE.EQ.'CR'.OR.IDTUBE.EQ.'MO')K1=1
      IF(K1.EQ.1)IDLINE(3)='  '
      IF(K1.EQ.1)IDLINE(4)='  '
      IF(IDTUBE.EQ.'W '.OR.IDTUBE.EQ.'AU')K1=3
      IF(K1.EQ.3)IDLINE(1)='  '
      IF(K1.EQ.3)IDLINE(2)='  '
      DO 10 I=1,7
      IF(IDTUBE.EQ.IDTGT(I))GOTO 20
10    CONTINUE
      WRITE(6,100)
      STOP
20    I1=I
      N1=2*I1-1
      N2=N1+1
      OPEN(UNIT=3,NAME='TGTWR.DAT',TYPE='OLD',ACCESS='DIRECT',
     +  MAXREC=14,RECORDSIZE=11)
      READ(3'N1)(DATTGT(1,J),J=1,11)
      READ(3'N2)(DATTGT(2,J),J=1,11)
      CLOSE(UNIT=3)
      RETURN
100   FORMAT(/1X,'ERRER: THE NAME OF X-RAY TUBE TARGET YOU INPUT IS NO
     +T CORRECT !'/3X,'IT SHOULD BE ONE OF THE SEVEN TARGETS: SC, CR, MO
     +, RH, AG, W & AU.')
      END
```

```
      SUBROUTINE CHALIN(CINT,WV,IDLINE)
C
C     THIS SUBROUTINE CALCULATES THE CHARACTERISTIC LINE INTENSITY
C     OF AN X-RAY TUBE SPECTRUM USING THE NBS ALGORITHM.
C     (UNIT: PHOTONS/E/STRD)
C
C     NBS      24-JUL-1984
C
      COMMON K15
      COMMON /TUBE2/IDTUBE,VOLT,TOFAGL,WINTHI
      CALL ATNUM(IDTUBE,IZ)
      Z=FLOAT(IZ)
      IF(IDLINE.EQ.'KA')FZ=3.22E6/(9.76E4+Z**4)-.39
      IF(IDLINE.EQ.'KB')FZ=5.13E5/(2.05E5+Z**4)-.014
      IF(IDLINE.EQ.'LA')FZ=2.02E7/(2.65E6+Z**4)+.21
      IF(IDLINE.EQ.'LB')FZ=1.76E7/(6.05E6+Z**4)-.09
      U=WV*VOLT/12.398
      R=EXP(-.5*((U-1.0)/(1.17*U+3.20))**2)
      RATIO=R*FZ*(U*ALOG(U)/(U-1.0)-1.0)
      CALL CTNLIN(HINT,WV)
      CINT=RATIO*HINT
      RETURN
      END



      SUBROUTINE SBATWT(NAME,ATWT)
C
C     THIS SUBROUTINE PROVIDES THE ATOMIC WEIGHT WHEN A
C     CORRESPONDING ELEMENT NAME IS GIVEN.
C
C     NBS      04-SEP-1984
C
      DIMENSION AW(94)
      DATA AW/1.00797,4.0026,6.939,9.0122,10.811,12.01115,14.0067,
     1 15.9994,18.9984,20.183,22.9898,24.312,26.9815,28.086,30.9738,
     1 32.064,35.453,39.948,39.102,40.08,44.956,47.90,50.942,51.996,
     1 54.938,55.847,58.933,58.71,63.54,65.37,69.72,72.59,74.922,78.96,
     1 79.909,83.80,85.47,87.62,88.905,91.22,92.906,95.94,98.0,101.07,
     1 102.905,106.4,107.870,112.40,114.82,118.69,121.75,127.60,
     1 126.904,131.30,132.905,137.34,138.91,140.12,140.907,144.24,147.0,
     1 150.35,151.96,157.25,158.924,162.50,164.930,167.26,168.934,
     1 173.04,174.97,178.49,180.948,183.85,186.2,190.2,192.2,195.09,
     1 196.967,200.59,204.37,207.19,208.980,210.0,210.0,222.0,223.0,
     1 226.0,227.0,232.038,231.0,238.04,237.0,242.0/
      CALL ATNUM(NAME,IZ)
      ATWT=AW(IZ)
      RETURN
      END
```

```
      REAL FUNCTION MAC(INAM,WV)
C
C     THIS SUBROUTINE GENERATES MASS ABSORPTION COEFFICIENTS
C     AT A GIVEN WAVELENGTH FOR VARIOUS ELEMENTS ACCORDING
C     TO HEINRICH.
C
C     NBS     04-SEP-84
C
      DIMENSION C1(9),C2(9),C3(9),EC(9),CN(4),R(10)
      DIMENSION D1(4),D2(4),D3(4)
      DATA C1/-.0397931,-.0339160,-.0865397,-.2283427,1.251788,
     +        .8349031,.4422173,.2514096,.2729506/
      DATA C2/2.423000,2.825262,3.323153,4.311724,-7.837999,
     +        -4.149247,-.9792409,.9319132,.6889060/
      DATA C3/5.509104,9.035256,10.25054,12.00253,-11.58026,
     +        -3.338016,3.153478,8.035612,7.424300/
      DATA CN(3),CN(4)/2.6,2.22/
      DATA R/1.0,1.0,1.17,1.63,1.0,1.16,1.4,1.621,1.783,1.0/
      DATA D1/-.2322294,-.2544711,.2562163,1.359165/
      DATA D2/4.070053,4.769245,1.15119,-9.492116/
      DATA D3/-6.220746,-10.37878,-5.684848,18.64081/
      CALL ATNUM(INAM,IZ)
      E=12.398/WV
      ZI=IZ
      ZL=ALOG(ZI)
      DO 10 I=1,9
      EC(I)=EXP(C1(I)*ZL*ZL+C2(I)*ZL-C3(I))
10    CONTINUE
      CN(1)=EXP(-.0045522*ZL*ZL-.0068535*ZL+1.070181)
      CN(2)=2.73
      IF(IZ.LT.42)GOTO 20
      CN(2)=EXP(-.1131595*ZL*ZL+.8368829*ZL-.5459687)
20    CONTINUE
      DO 40 M=1,10
      IF(M.EQ.10)GOTO 30
      IF(E.LT.EC(M))GOTO 40
30    MI=M-M/3-M/4-M/7
      C=EXP(D1(MI)*ZL*ZL+D2(MI)*ZL+D3(MI))/R(M)
      MAC=C*WV**CN(MI)
      RETURN
40    CONTINUE
      END
```

```
      REAL FUNCTION MU(INAM,WV)
C
C     THIS SUBROUTINE GENERATES MASS ABSORPTION COEFFICIENTS AT
C     A GIVEN WAVELENGTH FOR VARIOUS ELEMENTS ACCORDING TO
C     LEROUX ALGORITHM (1979 VERSION).
C
C     NBS     04-SEP-1984
C
      IMPLICIT INTEGER (I,J)
      IMPLICIT REAL (A-H,K-Z)
      CALL ATNUM(INAM,IZ)
      E=12.3981/WV
      OPEN(UNIT=3,NAME='MACPRM.DAT',TYPE='OLD',ACCESS='DIRECT',
     1 MAXREC=94,RECORDSIZE=24)
      READ(3'IZ) C,K,NK,EP,CK1,NCK1,L1,NL1,L2,NL2,L3,NL3,M1,NM1,
     1 M2,NM2,M3,NM3,M4,NM4,M5,NM5,N1,NN1
      CLOSE(UNIT=3)
      IF(E.GT.K) GO TO 30
      IF(E.GT.L1) GO TO 40
      IF(E.GT.L2) GO TO 50
      IF(E.GT.L3) GO TO 60
      IF(E.GT.M1) GO TO 70
      IF(E.GT.M2) GO TO 80
      IF(E.GT.M3) GO TO 90
      IF(E.GT.M4) GO TO 100
      IF(E.GT.M5) GO TO 110
      IF(E.LT.N1) GO TO 120
      MU=C*N1*WV**NN1
      GO TO 150
30    IF(IZ.GT.57) GO TO 120
      IF(E.LT.EP) GO TO 35
      MU=C*K*WV**NK
      GO TO 150
35    MU=CK1*WV**NCK1
      GO TO 150
40    MU=C*L1*WV**NL1
      GO TO 150
50    MU=C*L2*WV**NL2
      GO TO 150
60    MU=C*L3*WV**NL3
      GO TO 150
70    MU=C*M1*WV**NM1
      GO TO 150
80    MU=C*M2*WV**NM2
      GO TO 150
90    MU=C*M3*WV**NM3
      GO TO 150
100   MU=C*M4*WV**NM4
      GO TO 150
110   MU=C*M5*WV**NM5
      GO TO 150
120   MU=0.
150   RETURN
      END
```

```
      PROGRAM CALCOMP
C
C       THIS IS A REVISION OF VERSION 1 OF A FUNDAMENTAL PARAMETER
C      COMPUTER PROGRAM FOR CORRECTION OF INTERELEMENT EFFECTS FOR
C      QUANTITATIVE X-RAY SPACTROMETRY. THE ORIGINAL PROGRAM WAS
C      WRITTEN BY R.M.ROUSSEAU OF THE GEOLOGICAL SURVEY OF CANADA
C      (GSC) AND CONTAINS THE PROGRAMS ALPHA AND CARECAL WHICH WERE
C      EXTENSIVELY MODIFIED AT NBS. THE NBSGSC PROGRAM CONTAINS THE
C      COMPREHENSIVE LACHANCE ALGORITHM(COLA) FOR CORRECTION OF INTER-
C      ELEMENT EFFECTS.
C       CALCO IS A REVISION OF ALPHA FOR CALCULATING THEORETICAL ALPHA
C      COEFFICIENTS, AND CALCOMP IS A REVISION OF CARECAL FOR CALCULA-
C      TING CONCENTRATIONS IN ANALYTE SPECIMENS.
C
C      OVERLAY STRUCTURE OF CALCOMP :
C        MAIN PROGRAM-----CALCOMP
C        SUBROUTINE-------DATAIN,CALRI,GETERR,SVLSF2,SLE
C                  *
C      AUTHORS: G.Y. TAO  AND P.A. PELLA          DATE: 07-SEP-1984
C        CENTER FOR ANALYTICAL CHEMISTRY, NATIONAL BUREAU OF STANDARDS
C        GAITHERSBURG MD 20899 U.S.A.
C              AND R.M.ROUSSEAU
C        GEOLOGICAL SURVEY OF CANADA, OTTAWA, CANADA K1A-0E8
C
C      * GUEST RESEARCHER FROM SHANGHAI INSTITUTE OF CERAMICS,
C        ACADEMIA SINICA, THE PEOPLE'S REPUBLIC OF CHINA
C
      REAL IP(13),IX(20,13),IS(20,13)
      DIMENSION IDATE(5),ITIME(4),A1(13,13),A2(12,12),A3(12,12),
     +          AIJK(12,12,12),CS(20,13),CIM(13),SCI(13),CX(20,13),
     +          TOT(20),CX1(20,13),RX(20,13),RX1(20,12)
      DOUBLE PRECISION NOA(13),NOA1(13),NS(20),NX(20)
      COMMON K1,N6,N,M,M1,K2,KK1,KK6
      COMMON /DATSUB/CS,IS,IX,NS,IP
      COMMON /COESUB/A1,A2,A3,AIJK
      COMMON /CALSUB/RX,RX1
      COMMON /GETSUB/NOA,NOA1,NX,CX,TOT
      DATA KK6/'N '/
      CALL DATE(IDATE)
      CALL TIME(ITIME)
      WRITE(6,500)IDATE,ITIME
      WRITE(6,510)
      READ(5,*)K1
      CALL DATAIN
      N2=N6-1
      WRITE(6,520)
      READ(5,530)KK7
      IF(KK7.EQ.'Y ')WRITE(6,540)
      IF(KK7.EQ.'Y ')READ(5,*)D
      D=D*1.0E-6
      IF(K2.EQ.2)GOTO 45
      DO 40 I=1,M
      IF(KK1.EQ.'Y ')J7=0
      DO 40 J=1,N6
      DO 10 I8=1,N
      IF(NOA(J).EQ.NOA1(I8))GOTO 20
10    CONTINUE
      GOTO 30
20    IF(KK1.EQ.'Y ')J7=J7+1
      IF(KK7.EQ.'Y ')IP(J)=IP(J)/(1.0-D*IP(J))
      IF(KK7.EQ.'Y ')IX(I,J)=IX(I,J)/(1.0-D*IX(I,J))
      RX(I,J)=IX(I,J)/IP(J)
      IF(KK1.EQ.'Y ')RX1(I,J7)=RX(I,J)
```

```
      GOTO 40
30    RX(I,J)=IX(I,J)
40    CONTINUE
      GOTO 55
45    IF(KK7.EQ.'N ')GOTO 50
      DO 46 I=1,M1
      DO 46 J=1,N6
      DO 46 I8=1,N
      IF(NOA(J).EQ.NOA1(I8))IS(I,J)=IS(I,J)/(1.0-D*IS(I,J))
46    CONTINUE
      DO 48 I=1,M
      DO 48 J=1,N6
      DO 48 I8=1,N
      IF(NOA(J).EQ.NOA1(I8))IX(I,J)=IX(I,J)/(1.0-D*IX(I,J))
48    CONTINUE
50    CALL CALRI
55    WRITE(6,545)
      DO 200 L=1,M
      IF(KK1.EQ.'Y ')WRITE(6,550)NX(L),(NOA1(I),RX1(L,I),I=1,N)
      IF(KK1.EQ.'N ')WRITE(6,550)NX(L),(NOA(I),RX(L,I),I=1,N)
      DO 60 I=1,N6
      CIM(I)=0.0
      IF(RX(L,I).LT.0.0)RX(L,I)=0.0
      CX(L,I)=RX(L,I)
60    CONTINUE
      L1=1
65    DO 130 I=1,N6
      IF(KK1.EQ.'N ')GOTO 90
      DO 70 I8=1,N
      IF(NOA(I).EQ.NOA1(I8))GOTO 90
70    CONTINUE
      GOTO 130
90    SCI(I)=0.0
      IF(ABS(CX(L,I)-CIM(I)).LE.0.0001)GOTO 130
      CM=0.0
      DO 100 I9=1,N6
      CM=CM+CX(L,I9)
100   CONTINUE
      CM=CM-CX(L,I)
      DO 110 J=1,N6
      IF(K1.EQ.3)SCI(I)=SCI(I)+CX(L,J)*A1(I,J)
      IF(K1.EQ.2)SCI(I)=SCI(I)+CX(L,J)*(A1(I,J)+A2(I,J)*CM)
      IF(K1.EQ.1)SCI(I)=SCI(I)+CX(L,J)*(A1(I,J)+A2(I,J)*CM/
     +  (1.0+A3(I,J)*(1.0-CM)))
110   CONTINUE
      IF(K1.EQ.3)GOTO 125
      DO 120 J=1,N2
      KK=J+1
      DO 120 K=KK,N6
      SCI(I)=SCI(I)+AIJK(I,K,J)*CX(L,J)*CX(L,K)
120   CONTINUE
125   CIM(I)=CX(L,I)
      CX(L,I)=RX(L,I)*(1.0+SCI(I))
130   CONTINUE
      DO 160 I=1,N6
      IF(KK1.EQ.'N ')GOTO 150
      DO 140 I8=1,N
      IF(NOA(I).EQ.NOA1(I8))GOTO 150
140   CONTINUE
      GOTO 160
150   IF(ABS(CX(L,I)-CIM(I)).LE.0.0001)GOTO 160
      GOTO 170
160   CONTINUE
      GOTO 180
```

```
170      IF(L1.LE.10)L1=L1+1
         IF(L1.LE.10)GOTO 65
         IF(L1.GT.10)PAUSE'NO. OF ITERATION > 10'
180      TOT(L)=0.0
         DO 190 I9=1,N6
         CX1(L,I9)=CX(L,I9)*100.0
         CX(L,I9)=AINT(1.0E4*CX(L,I9)+.5)/100.0
         TOT(L)=TOT(L)+CX(L,I9)
190      CONTINUE
         WRITE(6,560)L1,(NOA(I),CX1(L,I),I=1,N6)
         WRITE(6,570)TOT(L)
200      CONTINUE
         WRITE(6,572)(NOA(I),I=1,N6)
         DO 210 L=1,M
         WRITE(6,574)NX(L),TOT(L),(CX1(L,I),I=1,N6)
210      CONTINUE
         WRITE(6,580)
         READ(5,530)KK5
         IF(KK5.EQ.'Y ')CALL GETERR
         IF(M1.EQ.1.OR.K2.EQ.1)GOTO 220
         WRITE(6,590)
         READ(5,530)KK6
         IF(KK6.EQ.'Y ')GOTO 50
220      WRITE(6,600)
         STOP
500      FORMAT(///1X,'DATE:  ',5A2,6X,'TIME:  ',4A2/)
510      FORMAT(1X,'WHAT TYPE OF UNKNOWNS DO YOU WISH TO ANALYZE :'/
     +   3X,'1-ELEMENT SYSTEM    2-OXIDE SYSTEM    3-FUSED DISK SYSTEM  ?
     +   ',$)
520      FORMAT(1X,'DO YOU WANT TO CORRECT INTENSITIES FOR DEAD TIME (Y/N
     +) ?  ',$)
530      FORMAT(A1)
540      FORMAT(1X,'INPUT THE DEAD TIME IN MICROSECONDS :  ',$)
545      FORMAT(/' -----RESULTS OF LAST ITERATION-----'/)
550      FORMAT(/1X,'SMP.NO.=',A8,2X,'R=',6(A8,F8.5,1X)/21X,6(A8,F8.5,
     +   1X))
560      FORMAT(13X,'L=',I2,2X,'C=',6(A8,F7.3,1H%,1X)/21X,6(A8,F7.3,
     +   1H%,1X)/21X,A8,F7.3,1H%)
570      FORMAT(19X,'TOTAL=',F7.2,1H%/)
572      FORMAT(//45X,'TABULATION OF RESULTS (%)'//
     +   1X,'SMP.NO.   TOTAL   ',13A8)
574      FORMAT(/1X,A8,1X,F7.2,13(F7.3,1X))
580      FORMAT(///1X,'DO YOU WISH TO COMPARE THESE RESULTS WITH OTHER P
     +REVIOUSLY KNOWN VALUES FOR THESE SPECIMENS (Y/N) ?  ',$)
590      FORMAT(//1X,'DO YOU WANT TO TRY ANOTHER TYPE OF CALIBRATION CURV
     +E (Y/N) ?  ',$)
600      FORMAT(///)
         END
```

```
      SUBROUTINE DATAIN
C
C     MOST OF THE INPUT DATA REQUIRED FOR CALCULATING CONCANTRATIONS
C     IS HANDLED BY THIS SUBROUTINE.
C
C     NBS        05-SEP-1984
C
      REAL IP(13),IX(20,13),IS(20,13)
      DIMENSION A1(13,13),A2(12,12),A3(12,12),AIJK(12,12,12),
     +          NAMFIL(5),CS(20,13)
      DOUBLE PRECISION NOA(13),NOA1(13),NS(20),NX(20)
      COMMON K1,N6,N,M,M1,K2,KK1
      COMMON /DATSUB/CS,IS,IX,NS,IP
      COMMON /COESUB/A1,A2,A3,AIJK
      COMMON /GETSUB/NOA,NOA1,NX
      WRITE(6,500)
      READ(5,510)KK1
      IF(KK1.EQ.'Y ')WRITE(6,520)
      IF(KK1.EQ.'Y ')READ(5,*)N6,N,M
      IF(KK1.EQ.'N ')WRITE(6,530)
      IF(KK1.EQ.'N ')READ(5,*)N,M
      IF(KK1.EQ.'N ')N6=N
      IF(KK1.EQ.'Y ')WRITE(6,540)
      IF(KK1.EQ.'Y ')READ(5,550)(NOA(I),I=1,N6)
      WRITE(6,560)
      READ(5,550)(NOA1(I),I=1,N)
      IF(KK1.EQ.'Y ')GOTO 20
      DO 10 I=1,N6
      NOA(I)=NOA1(I)
10    CONTINUE
20    WRITE(6,570)
      READ(5,*)K4
      IF(K4.EQ.1)GOTO 30
      WRITE(6,580)
      IF(K1.EQ.1)READ(5,*)((A1(I,J),J=1,N6),(A2(I,J),J=1,N6),
     +(A3(I,J),J=1,N6),((AIJK(I,J,K),K=1,N6),J=1,N6),I=1,N6)
      IF(K1.EQ.2)READ(5,*)((A1(I,J),J=1,N6),(A2(I,J),J=1,N6),
     +((AIJK(I,J,K),K=1,N6),J=1,N6),I=1,N6)
      IF(K1.EQ.3)READ(5,*)((A1(I,J),J=1,N6),I=1,N6)
      GOTO 50
30    WRITE(6,590)
      READ(5,600)NAMFIL
      CALL ASSIGN(3,NAMFIL,10)
      IF(K1.EQ.1)READ(3,*,ERR=40)((A1(I,J),J=1,N6),(A2(I,J),J=1,N6),
     +(A3(I,J),J=1,N6),((AIJK(I,J,K),K=1,N6),J=1,N6),I=1,N6)
      IF(K1.EQ.2)READ(3,*,ERR=40)((A1(I,J),J=1,N6),(A2(I,J),J=1,N6),
     +((AIJK(I,J,K),K=1,N6),J=1,N6),I=1,N6)
      IF(K1.EQ.3)READ(3,*,ERR=40)((A1(I,J),J=1,N6),I=1,N6)
40    CALL CLOSE(3)
50    WRITE(6,610)
      READ(5,*)K2
      IF(K2.EQ.2)WRITE(6,620)
      IF(K2.EQ.2)READ(5,*)M1
      IF(K2.EQ.2)GOTO 70
      IF(KK1.EQ.'Y ')WRITE(6,630)
      IF(KK1.EQ.'N ')WRITE(6,635)
      DO 60 I=1,N6
      DO 55 I8=1,N
      IF(NOA(I).EQ.NOA1(I8))GOTO 57
55    CONTINUE
      GOTO 60
57    WRITE(6,640)NOA(I)
      READ(5,*)IP(I)
```

```
60      CONTINUE
        GOTO 100
70      WRITE(6,650)
        DO 80 I=1,M1
        WRITE(6,660)I
        READ(5,670)NS(I)
80      CONTINUE
        WRITE(6,680)
        DO 90 I=1,M1
        WRITE(6,690)I,NS(I)
        READ(5,*)(CS(I,J),J=1,N6)
90      CONTINUE
        IF(KK1.EQ.'Y ')WRITE(6,695)
        IF(KK1.EQ.'N ')WRITE(6,697)
        DO 96 I=1,M1
        WRITE(6,690)I,NS(I)
        READ(5,*)(IS(I,J),J=1,N6)
96      CONTINUE
100     WRITE(6,700)
        DO 110 I=1,M
        WRITE(6,660)I
        READ(5,670)NX(I)
110     CONTINUE
        IF(KK1.EQ.'Y ')WRITE(6,710)
        IF(KK1.EQ.'N ')WRITE(6,720)
        DO 120 I=1,M
        WRITE(6,690)I,NX(I)
        READ(5,*)(IX(I,J),J=1,N6)
120     CONTINUE
        RETURN
500     FORMAT(1X,'DO YOU WANT TO INPUT KNOWN CONCENTRATIONS OF UNANALYZ
     +ED ELEMENTS (Y/N)?  ',$)
510     FORMAT(A1)
520     FORMAT(1X,'INPUT N6(NUMBER OF ALL CONSTITUENTS), N(NUMBER OF ANA
     +LYTES) AND'/3X,'M(NUMBER OF SPECIMENS TO BE ANALYZED) :',10X,$)
530     FORMAT(1X,'INPUT N(NUMBER OF ANALYTES) & M(NUMBER OF SPECIMENS T
     +O BE ANALYZED) :  ',$)
540     FORMAT(' INPUT NAMES OF CONSTITUENTS(XXXXXXXX)(MAX.=8/LINE) :'/)
550     FORMAT(8A8)
560     FORMAT(1X,'INPUT NAMES OF ANALYTES(XXXXXXXX)(MAX.=8/LINE) :'/)
570     FORMAT(' DO YOU WANT TO INPUT ALPHA COEFFICIENTS BY: 1-DATAFILE
     +  2-KEYBOARD  ?  ',$)
580     FORMAT(1X,'TYPE IN THE ALPHA COEFFICIENTS :'/)
590     FORMAT(1X,'INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX)
     + :  ',$)
600     FORMAT(5A2)
610     FORMAT(' WHAT TYPE OF STANDARDS ARE AVAILABLE: 1-PURE STANDARDS
     +  2-MULTIELEMENT STANDARDS  ?  ',$)
620     FORMAT(1X,'INPUT M1(NUMBER OF STANDARDS)' :  ',$)
630     FORMAT(1X,'INPUT NET PURE INTENSITIES FOR EACH ANALYTE FOLLOWED
     +BY A PERIOD AND'/3X,'ENTER 0.0 FOR EACH UNANALYZED ELEMENT:'/)
635     FORMAT(1X,'INPUT NET PURE INTENSITIES FOR EACH ANALYTE FOLLOWED
     +BY A PERIOD :'/)
640     FORMAT(2X,A2,4X,$)
650     FORMAT(1X,'INPUT I.D. OF STANDARDS (<=8 CHARACTERS) :'/)
660     FORMAT(2X,'I=',I2,4X,$)
670     FORMAT(A8)
680     FORMAT(' INPUT CONCENTRATIONS(WEIGHT FRACTION) OF STANDARDS :'/)
690     FORMAT(2X,'I=',I2,4X,A8,2X,$)
695     FORMAT(1X,'INPUT NET INTENSITIES FOLLOWED BY A PERIOD FOR THE AN
     +ALYTE ELEMENTS IN STANDARDS AND'/3X,'ENTER 0.0 FOR EACH UNANALYZED
     + ELEMENT:'/)
697     FORMAT(1X,'INPUT NET INTENSITIES FOLLOWED BY A PERIOD FOR THE AN
     +ALYTE ELEMENTS IN STANDARDS :')
```

```
700     FORMAT(1X,'INPUT I.D. OF SPECIMENS TO BE ANALYZED :'/)
710     FORMAT(1X,'INPUT NET INTENSITIES FOR ANALYTES IN SPECIMENS AND'/
     +3X,'ENTER CONCENTRATIONS(WEIGHT FRACTION) FOR UNANALYZED ELEMENTS:
     +' /)
720     FORMAT(' INPUT NET INTENSITIES OF SPECIMENS TO BE ANALYZED :'/)
        END
```

```
      SUBROUTINE CALRI
C
C     THIS SUBROUTINE CALCULATES RELATIVE INTENSITIES OF ANALYTE
C     SPECIMENS USING MULTIELEMENT STANDARD(S) AND THE COLA
C     EQUATION.
C
C     NBS      05-SEP-1984
C
      REAL IP1(20,13),IS(20,13),IP11(20,13),IPP(12),IP(13),IX(20,13)
      DIMENSION SCI(13),CS(20,13),A1(13,13),A2(12,12),A3(12,12),
     + AIJK(12,12,12),RS(20,13),RS1(20,12),RX(20,13),RX1(20,12)
      DOUBLE PRECISION NOA(13),NOA1(13),NS(20),
     + X(20),Y(20),S(3),A(12,3),AA(11,3)
      COMMON K1,N6,N,M,M1,K2,KK1,KK6
      COMMON /DATSUB/CS,IS,IX,NS
      COMMON /COESUB/A1,A2,A3,AIJK
      COMMON /LSFSUB/X,Y
      COMMON /CALSUB/RX,RX1
      COMMON /GETSUB/NOA,NOA1
      EQUIVALENCE (X(1),IP11(1,1)),(Y(1),IP11(1,3)),(A(1,1),IP11(1,5))
     + ,(AA(1,1),IP11(1,9)),(IP1,RX),(RS1,RX1)
      IF(KK6.EQ.'Y ')GOTO 210
      N2=N6-1
      DO 90 L=1,M1
      IF(KK1.EQ.'Y ')J7=0
      DO 90 I=1,N6
      IF(KK1.EQ.'N ')GOTO 30
      DO 10 I8=1,N
      IF(NOA(I).EQ.NOA1(I8))GOTO 20
10    CONTINUE
      GOTO 90
20    J7=J7+1
30    SCI(I)=0.0
      CM=0.0
      DO 40 I9=1,N6
      CM=CM+CS(L,I9)
40    CONTINUE
      CM=CM-CS(L,I)
      DO 50 J=1,N6
      IF(K1.EQ.3)SCI(I)=SCI(I)+CS(L,J)*A1(I,J)
      IF(K1.EQ.2)SCI(I)=SCI(I)+CS(L,J)*(A1(I,J)+A2(I,J)*CM)
      IF(K1.EQ.1)SCI(I)=SCI(I)+CS(L,J)*(A1(I,J)+A2(I,J)*CM/
     + (1.0+A3(I,J)*(1.0-CM)))
50    CONTINUE
      IF(K1.EQ.3)GOTO 70
      DO 60 J=1,N2
      KK=J+1
      DO 60 K=KK,N6
      SCI(I)=SCI(I)+AIJK(I,K,J)*CS(L,J)*CS(L,K)
60    CONTINUE
70    RS(L,I)=CS(L,I)/(1.0+SCI(I))
      IF(RS(L,I).EQ.0.0)GOTO 80
      IP1(L,I)=IS(L,I)/RS(L,I)
80    IF(KK1.EQ.'Y ')RS1(L,J7)=RS(L,I)
      IF(KK1.EQ.'Y ')IP11(L,J7)=IP1(L,I)
90    CONTINUE
      IF(KK6.EQ.'Y ')GOTO 160
      WRITE(6,500)
      READ(5,510)KK3
      IF(KK3.EQ.'N ')GOTO 160
      IF(KK1.EQ.'Y ')WRITE(6,520)(NOA1(J),J=1,N)
      IF(KK1.EQ.'N ')WRITE(6,520)(NOA(J),J=1,N)
      DO 100 I=1,M1
```

```
      IF(KK1.EQ.'Y ')WRITE(6,530)NS(I),(RS1(I,J),J=1,N)
      IF(KK1.EQ.'N ')WRITE(6,530)NS(I),(RS(I,J),J=1,N)
100   CONTINUE
      IF(KK1.EQ.'Y ')J7=0
      DO 140 I=1,N6
      M11=M1
      DO 110 I8=1,N
      IF(NOA(I).EQ.NOA1(I8))GOTO 120
110   CONTINUE
      GOTO 140
120   IF(KK1.EQ.'Y ')J7=J7+1
      IP(I)=0.0
      DO 130 L=1,M1
      IF(CS(L,I).EQ.0.0)K11=1
      IF(CS(L,I).EQ.0.0)M11=M11-1
      IF(CS(L,I).EQ.0.0)GOTO 130
      IP(I)=IP(I)+IP1(L,I)
130   CONTINUE
      IF(K11.NE.1)IP(I)=IP(I)/FLOAT(M1)
      IF(K11.EQ.1)IP(I)=IP(I)/FLOAT(M11)
      IF(K11.EQ.1)K11=2
      IF(KK1.EQ.'Y ')IPP(J7)=IP(I)
140   CONTINUE
      IF(KK1.EQ.'Y ')WRITE(6,540)(NOA1(J),J=1,N)
      IF(KK1.EQ.'N ')WRITE(6,540)(NOA(J),J=1,N)
      DO 150 I=1,M1
      IF(KK1.EQ.'Y ')WRITE(6,550)NS(I),(IP11(I,J),J=1,N)
      IF(KK1.EQ.'N ')WRITE(6,550)NS(I),(IP1(I,J),J=1,N)
150   CONTINUE
      IF(KK1.EQ.'Y ')WRITE(6,555)(IPP(J),J=1,N)
      IF(KK1.EQ.'N ')WRITE(6,555)(IP(J),J=1,N)
160   IF(M1.NE.1)GOTO 210
      WRITE(6,557)
      K3=3
      GOTO 215
210   WRITE(6,560)
      READ(5,*)K3
215   IF(K3.EQ.1.OR.K3.EQ.3)N9=1
      IF(K3.EQ.2.OR.K3.EQ.4)N9=2
      WRITE(6,570)
      READ(5,510)KK4
      IF(KK1.EQ.'Y  )J7=0
      DO 270 L=1,N6
      IF(KK1.EQ.'N ')GOTO 240
      DO 220 I8=1,N
      IF(NOA(L).EQ.NOA1(I8))GOTO 230
220   CONTINUE
      GOTO 270
230   J7=J7+1
240   DO 250 I=1,M1
      X(I)=IS(I,L)
      Y(I)=RS(I,L)
250   CONTINUE
      CALL SVLSF2(S,K3,N9,M1)
      DO 260 I=1,3
      A(L,I)=S(I)
      IF(KK1.EQ.'Y ')AA(J7,I)=A(L,I)
260   CONTINUE
270   CONTINUE
      DO 320 L=1,M
      IF(KK1.EQ.'Y ')J7=0
      DO 320 I=1,N6
      IF(KK1.EQ.'N ')GOTO 300
      DO 280 I8=1,N
```

```
      IF(NOA(I).EQ.NOA1(I8))GOTO 290
280   CONTINUE
      GOTO 310
290   J7=J7+1
300   IF(IX(L,I).EQ.0.0)IX(L,I)=1.0E-20
      RX(L,I)=A(I,1)+A(I,2)*IX(L,I)+A(I,3)*IX(L,I)*IX(L,I)
      IF(KK1.EQ.'Y ')RX1(L,J7)=RX(L,I)
      GOTO 320
310   IF(KK1.EQ.'Y ')RX(L,I)=IX(L,I)
320   CONTINUE
      IF(KK4.EQ.'N ')RETURN
      WRITE(6,580)
      DO 330 I=1,N
      IF(KK1.EQ.'Y ')WRITE(6,590)NOA1(I),(AA(I,J),J=1,3)
      IF(KK1.EQ.'N ')WRITE(6,590)NOA(I),(A(I,J),J=1,3)
330   CONTINUE
      RETURN
500   FORMAT(1X,'DO YOU WANT TO PRINT OUT CALCULATED RELATIVE INTENSIT
     +IES OF STANDARDS &'/2X,' CALCULATED PURE INTENSITIES FROM STANDARD
     +S (Y/N) ? ',$)
510   FORMAT(A1)
520   FORMAT(/1X,'CALCULATED RELATIVE INTENSITIES OF STANDARDS :',/
     +  19X,12(1X,A8))
530   FORMAT(1X,'STD.NO.=',A8,2X,12(F8.5,1X))
540   FORMAT(/1X,'CALCULATED PURE INTENSITIES FROM STANDARDS :',/
     +  19X,12(1X,A8))
550   FORMAT(1X,'STD.NO.=',A8,2X,12F9.0)
555   FORMAT(/1X,'AVERAGE VALUES',4X,12F9.0)
557   FORMAT(/1X,'BECAUSE ONLY ONE STANDARD IS AVAILABLE, THE ONLY CHO
     +ICE FOR LSF CALIBRATION CURVE IS:  Y=A1*X.')
560   FORMAT(/1X,'WHAT TYPE OF LSF CURVES DO YOU WANT TO USE FOR CALIB
     +RATION :' /3X,'(1) Y=A0+A1*X       (2) Y=A0+A1*X+A2*X*X'
     +  /3X,'(3) Y=A1*X          (4) Y=A1*X+A2*X*X       ?   ',$)
570   FORMAT(' DO YOU WANT TO PRINT OUT LSF COEFFICIENTS (Y/N) :  ',$)
580   FORMAT(/15X,'TABULATION OF CALCULATED LSF COEFFICIENTS',/
     +  19X,'(X=MEAS.INT.  ;  Y=CALC.REL.INT.)',/)
590   FORMAT(1X,A8,2X,'A0=',E12.5,2X,'A1=',E12.5,2X,'A2=',E12.5)
      END
```

```
      SUBROUTINE GETERR
C
C     THIS SUBROUTINE COMPARES RESULTS FROM COLA WITH OTHER
C     PREVIOUSLY KNOWN VALUES.
C
C     NBS      05-SEP-1984
C
      DIMENSION CXT(20,13),CX(20,13),TOTT(20),EA(13),ER(13),
     + DIF(20,13),DIFR(20,13),TOT(20)
      DOUBLE PRECISION NX(20),NOA(13),NOA1(13)
      COMMON K1,N6,N,M,M1,K2,KK1,KK6
      COMMON /GETSUB/NOA,NOA1,NX,CX,TOT
      IF(KK6.EQ.'Y ')GOTO 45
      WRITE(6,500)
      DO 10 I=1,M
      WRITE(6,505)NX(I)
      READ(5,*)(CXT(I,J),J=1,N6)
10    CONTINUE
20    DO 40 L=1,M
      TOTT(L)=0.0
      DO 30 I=1,N6
      CXT(L,I)=AINT(1.0E4*CXT(L,I)+.5)/100.0
      TOTT(L)=TOTT(L)+CXT(L,I)
30    CONTINUE
40    CONTINUE
45    DO 80 I=1,N6
      EA(I)=0.0
      ER(I)=0.0
      IF(KK1.EQ.'N ')GOTO 60
      DO 50 I8=1,N
      IF(NOA(I).EQ.NOA1(I8))GOTO 60
50    CONTINUE
      GOTO 80
60    DO 70 L=1,M
      DIF(L,I)=CX(L,I)-CXT(L,I)
      IF(CXT(L,I).EQ.0.0)DIFR(L,I)=0.0
      IF(CXT(L,I).EQ.0.0)GOTO 70
      DIFR(L,I)=100.0*DIF(L,I)/CXT(L,I)
      EA(I)=EA(I)+ABS(DIF(L,I))
      ER(I)=ER(I)+100.0*ABS(DIF(L,I))/CXT(L,I)
70    CONTINUE
      EA(I)=EA(I)/FLOAT(M)
      ER(I)=ER(I)/FLOAT(M)
80    CONTINUE
      WRITE(6,510)(NOA(I),I=1,N6)
      DO 90 L=1,M
      WRITE(6,520)NX(L),TOTT(L),(CXT(L,I),I=1,N6)
      WRITE(6,530)TOT(L),(CX(L,I),I=1,N6)
      WRITE(6,540)(DIF(L,I),I=1,N6)
      WRITE(6,550)(DIFR(L,I),I=1,N6)
90    CONTINUE
      WRITE(6,560)(EA(I),I=1,N6)
      WRITE(6,570)(ER(I),I=1,N6)
      RETURN
500   FORMAT(1X,'ENTER KNOWN CONCENTRATIONS OF SPECIMENS :'/)
505   FORMAT(1X,'SMP.NO.=',A8,2X,$)
510   FORMAT(//45X,'TABULATION OF RESULTS (%)'//
     + 1X,'SMP.NO.   TOTAL   ',13A8)
520   FORMAT(/1X,A8,1X,F7.2,13(F7.2,1X))
530   FORMAT(10X,F7.2,13(F7.2,1X))
540   FORMAT(9X,'ABS.ERR.',13(F7.2,1X))
550   FORMAT(9X,'REL.ERR.',13(F7.2,1X))
560   FORMAT(//5X,'AVG.ABS.ERR.',13(F7.2,1X))

570   FORMAT(5X,'AVG.REL.ERR.',13(F7.2,1X))
      END
```

```
      SUBROUTINE SVLSF2(S,K1,N9,N)
C
C     THE SUBROUTINE PERFORMS A LEAST-SQUARES FIT FOR
C     SINGLE VARIABLE.
C
C     NBS     24-MAY-1984
C
      DIMENSION S(3),X(20),Y(20),A(3,4),T(5)
      DOUBLE PRECISION S,A,X,Y,T1,T2,T,S1,S2,S3,V,U,P1
      COMMON /LSFSUB/X,Y
      N10=N9+1
      N11=N9+2
      N12=N9*2+1
      IF(K1.EQ.1.OR.K1.EQ.2)GOTO 15
      T1=0.0
      IF(K1.EQ.4)T2=0.0
      S1=0.0
      IF(K1.EQ.4)S2=0.0
      IF(K1.EQ.4)S3=0.0
      DO 10 I=1,N
      IF(X(I).EQ.0.0)X(I)=1.0E-20
      T1=T1+X(I)*Y(I)
      IF(K1.EQ.4)T2=T2+X(I)*X(I)*Y(I)
      S1=S1+X(I)*X(I)
      IF(K1.EQ.4)S2=S2+X(I)**3
      IF(K1.EQ.4)S3=S3+X(I)**4
10    CONTINUE
      IF(K1.EQ.3)S(1)=0.0
      IF(K1.EQ.3)S(2)=T1/S1
      IF(K1.EQ.3)S(3)=0.0
      IF(K1.EQ.3)GOTO 70
      N10=N10-1
      N11=N11-1
      A(1,1)=S1
      A(1,2)=S2
      A(1,3)=T1
      A(2,1)=S2
      A(2,2)=S3
      A(2,3)=T2
      GOTO 55
15    DO 30 I=1,N12
      V=0.0
      U=0.0
      DO 20 J=1,N
      IF(X(J).EQ.0.0)X(J)=1.0E-20
      P1=X(J)**(I-1)
      U=U+P1
      IF(I.GT.N10)GOTO 20
      V=V+Y(J)*P1
20    CONTINUE
      T(I)=U
      IF(I.GT.N10)GOTO 30
      A(I,N11)=V
30    CONTINUE
      LL=0
      DO 50 I=1,N10
      DO 40 J=1,N10
      A(I,J)=T(J+LL)
40    CONTINUE
      LL=LL+1
50    CONTINUE
55    CALL SLE(S,A,N10)
      IF(K1.EQ.1)S(3)=0.0
```

```
      IF(K1.EQ.4)GOTO 60
      GOTO 70
60    N10=N10+1
      N11=N11+1
      S(3)=S(2)
      S(2)=S(1)
      S(1)=0.0
70    RETURN
      END


      SUBROUTINE SLE(S,A,N)
C
C     THIS SUBROUTINE IS USED TO SOLVE
C     SIMULTANEOUS LINEAR EQUATIONS
C
C     NBS     22-MAY-1984
C
      INTEGER P,Q,O
      DIMENSION A(3,4),S(4),O(3)
      DOUBLE PRECISION A,E,S,R
      N1=N+1
      DO 220 I=1,N
      P=I
      Q=1
      E=A(I,1)
      DO 120 J=I,N
      DO 100 K=1,N
      IF(ABS(A(J,K)).LE.ABS(E))GOTO 100
      E=A(J,K)
      Q=K
      P=J
100   CONTINUE
120   CONTINUE
      IF(ABS(E).GT.1.0E-30)GOTO 140
C     THE LARGEST ELEMENT IS EQUAL TO ZERO
      WRITE(6,260)
      STOP
C     TO CHANGE P-TH ROW WITH I-TH ROW
140   DO 160 K=1,N1
      S(K)=A(I,K)
      A(I,K)=A(P,K)
      A(P,K)=S(K)
160   CONTINUE
C     TO ZERO OUT Q-TH COLUMN
      DO 200 J=1,N
      IF(J.EQ.I)GOTO 200
      IF(A(J,Q).EQ.0.0)GOTO 200
      R=A(J,Q)/A(I,Q)
      DO 180 K=1,N1
      A(J,K)=A(J,K)-A(I,K)*R
180   CONTINUE
200   CONTINUE
      O(I)=Q
220   CONTINUE
      DO 240 I=1,N
      Q=O(I)
      S(Q)=A(I,N1)/A(I,Q)
240   CONTINUE
      RETURN
260   FORMAT(/1X,'NO UNIQUE SOLUTION')
      END
```

Appendix 2: Description of Symbols and Permanent Datafiles

2.1 List of Symbols and Variables in CALCO

(1) Main Program CALCO

Variable Names	Common Symbols	Remarks
A1(I,J)	α_1	Coefficient of element J on element I
A2(I,J)	α_2	Coefficient of element J on element I
A3(I,J)	α_3	Coefficient of element J on element I
AIJK(I,J,K)	α_{ijk}	Cross coefficient of elements J and K on element I
IDATE(5)		Date from computer's real-time clock
IELE(I)		Chemical symbol of analyte I
ITIME(4)		Time from computer's real-time clock
K1		Optional switch for analyzing: (1) element or (2) oxide or (3) fused disc system
K15		Optional switch for choosing: (1) Leroux or (2) Heinrich algorithm for calculating mass absorption coefficients
KK1		Optional switch for creating datafile for saving calculated alpha coefficients
N		Number of analytes
NAMFIL(5)		Datafile name for saving alpha coefficients
NE(I)		Number of the element atoms in the defined oxide formula for analyte I
NO(I)		Number of oxygen atoms in the defined oxide formula for analyte I

(2) Additional Variables in ALPHA

ALFA(I)	α'_{ij}	Coefficient α'_{ij} when $C_i = 0.3$, $C_j = 0.7$
C(5,3)	C_i	Concentration of hypothetical standards used to calculate alpha coefficients in element or oxide systems
CAM(I)		Mean concentration of analyte I in sample for fused disc system
CL(I,4)	λ_i, $\lambda_{i,ab}$, $\omega_i*(1-1/\gamma_i)$	Calculated wavelength of analyte line and its corresponding absorption edge, and product of fluorescent yield and jump ratio and atomic fraction of element I in its oxide
G(5)		Expression $(C_i/R_i-1)/C_j$
ICAS		Switch for calculating α'_{ij} or α'_{ijk}

IDTUBE		Chemical symbol of x-ray tube target
IE(I)		Intermediate variable
ISR(I)		Analyte line number (1-K_α, 2-K_β, 3-$L_{\alpha 1}$, 4-$L_{\beta 1}$, 5-$L_{\beta 2}$)
ITP	Ψ_1	X-ray incidence angle
ITS	Ψ_2	X-ray emergence angle
IZ(I)	Z	Atomic number of analyte I
K12		Optional switch used for different fused disk conditions: (1) Sample+ LI2B407; (2) sample+ LI2B407+ LIF; (3) sample+LiBO2.
KK2		Optional switch for printing out calculated alpha coefficients
KK5		Switch for using AL filter when analyzing Cr and Mn with Cr X-ray tube
MAC	$\mu_i(\lambda)$	Real function for calculating mass absorption coefficients with Heinrich algorithm
MU	$\mu_i(\lambda)$	Real function for calculating mass absorption coefficients with Leroux algorithm
N5,NAM		Intermediate Variables
RJM	$1-1/\gamma$	Jump Ratio
SW,SW1,SWDB		Intermediate Variables
SWDB1,SWLOI		Intermediate Variables
TP	CSC Ψ_1	Cosecant of incident angle Ψ_1
TS	CSC Ψ_2	Cosecant of emergence angle Ψ_2
UC(I,J)	$\mu_i(\lambda_j)$	Mass absorption coefficient of element I at wavelength λ_j
UCO(J)	$\mu_o(\lambda_j)$	Mass absorption coefficient of oxygen at wavelength, λ_j
VOLT		Voltage (KV) used in X-ray tube
XINT(2,300)		Wavelength and intensity of X-ray tube continuum
XINT1(2,11)		Wavelength and intensity of X-ray tube characteristic lines
Y	ω	X-ray fluorescent yield
Z		Intermediate variable

(3) Additional Variables in APAFD

CA	C_i	Concentration C_i used for fused disc system
CB	C_j	Concentration C_j used for fused disc system

CLOI	C_{LOI}	Loss of ignition treated as a concentration
F		Ratio of sample to fused disk weight
RA	R	Calculated relative intensity
UCF(J)	$\mu_F(\lambda)$	Mass absorption coefficient of flux at wavelength λ

(4) Additional Variables in BDCOEF

BETA(I)	$\beta_{ij}(\lambda_k)$	Intermediate variables
CF		Ratio of flux to fused disk weight
DELTA(I)	$\delta_{ij}(\lambda_k)$	Intermediate variables
DEN,PHIF,SBETA		Intermediate variables
SDELTA,T1,T2,T3		Intermediate variables
U(I)	$\mu_i(\lambda_k)$	Mass absorption coefficient of element I at wavelength λ_k
UE,UEI,UEJ		Intermediate variables
UF	$\mu_F(\lambda_k)$	Mass absorption coefficient of flux at wavelength λ_k
UO	$\mu_O(\lambda_k)$	Mass absorption coefficient of oxygen at wavelength λ_k
W		Intermediate variable
WV1	λ_k	Wavelength of primary spectrum
WV2	$I_o(\lambda_k)\Delta\lambda$	Integral intensity of primary spectrum at wavelength λ_k

(5) Additional Variables in TUBDAT

CINT	Calculated intensity of characteristic line emitted from X-ray tube with NBS algorithm
DATTGT(2,11)	Wavelength and intensity ratio of each L-series characteristic line to that of $L_{\alpha 1}$ line
DFSP(6)	Datafile name of x-ray tube spectrum
EDGE	Ending wavelength of primary spectrum
IDLINE(4)	Symbols of characteristic lines K_α, K_β, L_α, L_β
K11	Optional swtich for choosing: (1) calculated or (2) measured primary spectrum
KK11	Optional switch for printing out data of primary spectrum used
ND	Number of wavelength intervals (.02A) between wavelengths WVMIN and EDGE
RLA	Calculated intensity of L_α line emitted from x-ray tube

TOFAGL	ϕ	Take-off angle in x-ray tube
WINTHI		Window thickness of x-ray tube
WV	λ	A given x-ray wavelength
WVMIN	λ_{min}	Short wavelength limit of x-ray tube at a given voltage

(6) Additional Variables in CTNLIN

F		Intermediate variable
HINT	$I_o \Delta\lambda$	Integral intensity of primary spectrum
PSE,TB		Intermediate Variables
R	CSC ϕ	Cosecant of take-off angle in x-ray tube
Z		Conversion of IZ from integer to real mode

(7) Additional Variables in CHALIN

FZ,R,U		Intermediate Variables
RATIO		Calculated ratio of intensity of characteristic line to that of the corresponding continuum from x-ray tube

(8) Additional Variables in INFTGT

IDTGT(7)		Chemical symbols of seven commonly used X-ray tube targets

(9) Additional Variables in MAC

C		Coefficient in the expresion: $\mu_i(\lambda) = C_i * \lambda^{n_i}$
C1(9), C2(9), C3(9)		Coefficients for computing the absorption edge energies
CN(4)	n_i	The value of n in the above expression
D1(4),D2(4),D3(4)		Coefficients for computing the necessary value of C
E		Energy of the wavelength WV
ED(9)	E_{ab}	Energy of each absorption edge
INAM		Chemical symbol of a given element
MI		Number for selecting the proper coefficient for computing C

M	MI	M	MI
1	1	6	3
2	2	7	3
3	2	8	3
4	2	9	3
5	3	10	4

R(10)		Energy jump for each edge ZI
		Conversion of IZ from integer to real mode
ZL	LN(Z)	Logarithm of ZI

(10) Additional Variables in MACFUN

C	Coefficient in the expression: $\mu_i(\lambda) = C_i E_{i,ab} \lambda^{n_i}$
CK1	Coefficient in the expression: $\mu_i(\lambda) = C'_{ik} \lambda^{n_i}$
EP	Energy edge
K,L1,L2,L3	Energy of each absorption edge
M1,M2,M3,M4,,M5, N1	Energy of each absorption edge
NCK1,NK,NL1,NL2, NL3	The value of n in the above expression
NM1,NM2,NM3,NM4, NM5,NN1	The value of n in the above expression

(11) Additional Variables in AFIOX

AFOX	Atomic fraction of a given element in its oxide
AWE	Atomic weight of a given element
AWO	Atomic weight of oxygen

(12) Additional Variables in ABSEDG

C1(4),C2(4),C3(4)		Coefficients for computing the absorption edge energies
WV	λ_{ab}	Wavelength of absorption edge

(13) Additional Variables in CHAWV

D1(6),D2(6),D3(6)	Coefficients for computing the characteristic line wavelength
WV	Wavelength of characteristic line

WV		Wavelength of characteristic line

(14) Additional Variables in JUMRAT

JK(94)		Jump ratios for the absorption edge K
JL(94)		Jump ratios for absorption edge L
JUMP	$1-1/\gamma$	Jump ratio at a given absorption edge

(15) Additional Variables in Yield

OM1		Intermediate variable
Y	ω	X-ray fluorescence yield

(16) Additional Variable in ATNUM

ID(94)		Chemical symbols of the element (1-94)

(17) Additional Variables in SBATWT

AW(94)		Atomic weight of the elements (1-94)
ATWT		Atomic weight of a given element
NAME		Chemical symbol of a given element

2.2 List of Symbols and Variables in CALCOMP

(1) Main Program

Variable Names	Common Symbols	Remarks
A1(I,J)	α_1	Coefficient of element J on element I
A2(I,J)	α_2	Coefficient of element J on element I
A3(I,J)	α_3	Coefficient of element J on element I
AIJK(I,J,K)	α'_{ijk}	Cross coefficient of elements J and K on element I
CIM(I)		Intermediate concentration during interation process
CM		Concentration $Cm = 1-C_i = \Sigma\ C_j$
CS(M1,I)	C_i^s	Concentration of standard
CX(M,I)	C_i^x	Concentration calculated or fixed for unknown
CX1(M,I)	C_i^x	Concentration calculated or fixed for unknown
D		Dead time
IDATE(5)		Date from computer's real-time clock
IP(I)	I_i^p	Intensity of pure element I
IS(M1,I)	I_i^s	Intensity of standard
ITIME(4)		Time from computer's real-time clock
IX(M,I)	I_i^x	Intensity of unknown
K1		Optional switch for analyzing (1) element or (2) oxide, or (3) fused disk system
K2		Optional switch for using (1) pure or (2) multielement standard
KK5		Optional switch for obtaining error message
KK6		Optional switch for trying another type of calibration
KK7		Optional switch for dead time correction
M		Number of unknown(s)
M1		Number of standard(s)
N		Number of analytes
N6		Number of all constituents

NOA(I)		Chemical symbols of constituents
NOA1(I)		Chemical symbols of analytes
NS(I)		Identification of standard(s)
NX(I)		Identification of unknown(s)
RX(M,I)	R_i^x	Calculated relative intensity of unknown
RX1(M,I)	R_i^x	Calculated relative intensity of unknown
SCI(I)		Sum of terms $\alpha'_{ij}\ C_j$ and $\alpha'_{ijk}\ C_j\ C_k$
TOT(M)		Sum of concentrations calculated for unknown

(2) Additional Variables in DATAIN

K4	Optional switch for inputting coefficients by (1) datafile or (2) key-in on keyboard
KK1	Optional switch for using fixed concentrations
NAMFIL(5)	Datafile name of ALPHA coefficients

(3) Additional Variables in CALRI

A(I,3)	Calibration coefficient obtained with least squares fitting of R_i^s versus I_i^s
AA(I,3)	Calibration coefficient obtained with least squares fitting of R_i^s versus I_i^s
IP1(M1,I)	Calculated pure intensity from standard
IP11(M1,I)	Calculated pure intensity from standard
IP(I)	Average of calculated pure intensity from standards
IPP(I)	Average of calculated pure intensity from standards
K3	Optional switch for choosing a certain type of least squares fit for calibration: (1) Y=AO+A1*X; (2) Y=AO+A1*X+A2*X*X; (3) Y=A1*X; (4) Y=A1*X+A2*X*X
KK3	Optional switch for printing out calculated relative intensity of standard and pure intensity calculated from standard
KK4	Optional switch for printing out calibration coefficient
N9	Fitting exponent of least squares
RS(M1,I)	R_i^s Calculated relative intensity of standards

RS1(M1,I)	R_i^s	Calculated relative intensity of standards
S(3)		Coefficients of least squares fit
X(20)		Independent variables in least squares fit
Y(20)		Dependent variables in least squares fit

(4) Additional Variables in GETERR

CXT(M,I)		True concentration of unknowns
DIF(M,I)	A.R.	Absolute error of calculated concentration for unknowns
DIFR(M,I)	E.R.	Relative error of calculated concentration for unknowns
EA(I)		Average of absolute error of calculated concentration for unknown
ER(I)		Average of relative error of calculated concentration for unknown
TOTT(M)		Sum of true concentration for unknown

2.3 Description of Permanent Datafiles

Program	Function	Remarks
CREMAC	Create the datafile of MACPRM.DAT	Storing the parameters needed for computing mass absorption coefficients with the Leroux algorithm
RECREMAC	Print out the contents of the datafile MACPRM.DAT	For user to check if the contents of the datafile MACPRM.DAT are correct
WRTTGT	Create the datafile of TGTWR.DAT	Storing the wavelengths and intensity ratios of L-series lines to Lα line for seven types of x-ray tube targets
REWRTTGT	Print out the contents of the datafile TGTWR.DAT	For user to check if the contents of the datafile TGTWR.DAT are correct

3.1A is an example of the analysis of Cr-FE-NI ternary alloys where the measured W target X-ray tube spectral data at 45 kV [11] were used. A datafile named SDXT75.W45 was created before running the program CALCO. The program CALCO printed out calculated alpha coefficients, and could be saved, if desired, in a datafile if the answer to step 6 (figure 3) is 'Y'. An example of how to input the calculated alpha coefficients is given in 3.1B where only one multielement standard was employed.

3.2A is an example of the analysis of high temperature alloys using a CR target X-ray tube spectral data at 45 kV calculated from the NBS algorithm. The calculated alpha coefficients were saved in the datafile called ALLOY2.C45. In 3.2B, unknowns were analyzed where Cr, Mn, Fe, Ni, Cu, and Mo, were treated as the analytes, and C, Al, Si, V, Co, Nb are unanalyzed elements whose concentrations were previously known and entered as fixed concentrations.

(3) Examples of the analysis of cement treated as an oxide system are shown in 3.3A and 3.3.B, where among 12 constituents AL203, SI02, K20, CAO, TI02, MN203, and FE203 were the analytes, and the rest were entered as known constituents. In example 3.3B, two different calibration curves were used to obtain the concentrations of the unknown samples.

(4) Example 3.4A and 3.4B, illustrate the analysis of rock samples as fused disc specimens. In this system, the alpha coefficients are computed at an average composition level for the analyte in the range of interest. Also, a choice of three flux conditions can be selected by the user.

Appendix 3: Examples for Alloy, Oxide, and Fused Samples

3.1A Alpha Coefficient Calculation for Cr-Fe-Ni Alloy System Using Measured X-ray Tube Spectral Distribution from the Literature

```
$RUN CALCO


DATE:  02-OCT-84      TIME:  15:39:03

WHICH SYSTEM DO YOU WISH TO ANALYZE:
  1-ELEMENT SYSTEM  2-OXIDE SYSTEM  3-FUSED DISK SYSTEM  ?  1
INPUT NUMBER OF ANALYTES:  3
INPUT NAMES OF ANALYTES (XXS):  CR FE NI
WHAT MASS ABS. COEF. ALGORITHM DO YOU WANT TO USE :
  1-LEROUX ALGORITHM  2-HEINRICH ALGORITHM ?  2
DO YOU WANT TO CREATE A DATAFILE FOR SAVING CALCULATED ALPHA COEFFICIENTS (Y/N)?  N
FOR SAMPLE GEOMETRY, INPUT INCIDENCE & EMERGENCE ANGLES (DEGREE-XX):  63,33
INPUT THE CHARACTERISTIC LINE NUMBER YOU WISH TO MEASURE (1-KA, 2-KB, 3-LA1, 4-LB1, 5-LB2):
I= 1    CR    1
I= 2    FE    1
I= 3    NI    1
DO YOU WANT TO PRINT OUT CALCULATED ALPHA COEFFICIENTS(Y/N):  Y
WHICH X-RAY TUBE SPECTRAL DISTRIBUTION DO YOU PREFER:
  1-CALCULATED SPECTRUM FROM NBS ALGORITHM  ;  2-MEASURED SPECTRUM ?  2
DO YOU WANT TO PRINT OUT THE SPECTRAL DISTRIBUTION(Y/N) ?  Y
INPUT NAME OF X-RAY TUBE TARGET (XX) :  W
INPUT VOLTAGE(KV), TAKE-OFF ANGLE OF X-RAY FROM TUBE TARGET(DEGREE), AND
   WINDOW THICKNESS(MM) OF X-RAY TUBE :  45.0,26.0,1.0
INPUT THE DATAFILE NAME OF X-RAY TUBE SPECTRUM(XXXXXX.XXX) :  SDXT75.W45
INPUT TOTAL NUMBER OF WAVELENGTH INTERVALS FOR CONTINUUM (MAX.=300) :  117
```

MEASURED X-RAY TUBE SPECTRAL DISTRIBUTION

X-RAY TUBE TARGET: W KV: 45.0
TAKE-OFF ANGLE(DEGREE): 26.0 BE WINDOW THICKNESS(MM): 1.000

LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A
0.2700	0.0000E+00	0.2900	0.4400E+01	0.3100	0.1310E+02	0.3300	0.2090E+02	0.3500	0.2770E+02
0.3700	0.3270E+02	0.3900	0.3570E+02	0.4100	0.3780E+02	0.4300	0.3900E+02	0.4500	0.3930E+02
0.4700	0.3920E+02	0.4900	0.3880E+02	0.5100	0.3820E+02	0.5300	0.3740E+02	0.5500	0.3650E+02
0.5700	0.3570E+02	0.5900	0.3480E+02	0.6100	0.3400E+02	0.6300	0.3310E+02	0.6500	0.3220E+02
0.6700	0.3140E+02	0.6900	0.3040E+02	0.7100	0.2960E+02	0.7300	0.2880E+02	0.7500	0.2800E+02
0.7700	0.2720E+02	0.7900	0.2630E+02	0.8100	0.2560E+02	0.8300	0.2480E+02	0.8500	0.2400E+02
0.8700	0.2340E+02	0.8900	0.2260E+02	0.9100	0.2190E+02	0.9300	0.2120E+02	0.9500	0.2060E+02
0.9700	0.2000E+02	0.9900	0.1940E+02	1.0100	0.1910E+02	1.0300	0.1890E+02	1.0500	0.1890E+02
1.0700	0.1930E+02	1.0900	0.1960E+02	1.1100	0.1900E+02	1.1300	0.1840E+02	1.1500	0.1800E+02
1.1700	0.1740E+02	1.1900	0.1700E+02	1.2100	0.1760E+02	1.2300	0.2110E+02	1.2500	0.2140E+02
1.2700	0.2080E+02	1.2900	0.2020E+02	1.3100	0.1970E+02	1.3300	0.1910E+02	1.3500	0.1850E+02
1.3700	0.1800E+02	1.3900	0.1750E+02	1.4100	0.1700E+02	1.4300	0.1650E+02	1.4500	0.1600E+02
1.4700	0.1550E+02	1.4900	0.1500E+02	1.5100	0.1460E+02	1.5300	0.1410E+02	1.5500	0.1370E+02
1.5700	0.1330E+02	1.5900	0.1290E+02	1.6100	0.1250E+02	1.6300	0.1220E+02	1.6500	0.1180E+02
1.6700	0.1140E+02	1.6900	0.1110E+02	1.7100	0.1080E+02	1.7300	0.1040E+02	1.7500	0.1020E+02
1.7700	0.9800E+01	1.7900	0.9600E+01	1.8100	0.9300E+01	1.8300	0.9000E+01	1.8500	0.8700E+01
1.8700	0.8400E+01	1.8900	0.8200E+01	1.9100	0.7900E+01	1.9300	0.7700E+01	1.9500	0.7400E+01
1.9700	0.7200E+01	1.9900	0.7000E+01	2.0100	0.6700E+01	2.0300	0.6500E+01	2.0500	0.6200E+01
2.0700	0.6000E+01	2.0900	0.5800E+01	2.1100	0.5600E+01	2.1300	0.5400E+01	2.1500	0.5200E+01
2.1700	0.5000E+01	2.1900	0.4800E+01	2.2100	0.4700E+01	2.2300	0.4500E+01	2.2500	0.4400E+01
2.2700	0.4200E+01	2.2900	0.4000E+01	2.3100	0.3800E+01	2.3300	0.3700E+01	2.3500	0.3600E+01
2.3700	0.3500E+01	2.3900	0.3300E+01	2.4100	0.3200E+01	2.4300	0.3100E+01	2.4500	0.3000E+01
2.4700	0.2800E+01	2.4900	0.2700E+01	2.5100	0.2600E+01	2.5300	0.2500E+01	2.5500	0.2400E+01
2.5700	0.2300E+01	2.5900	0.2200E+01						

KA	KB	LA1	LB1	LB2	LB3	LB4	LG1	LG2	LG3	LL
0.0000	0.0000	1.4776	1.2818	1.2454	1.2627	1.3016	1.0986	1.0686	1.0620	1.6782
0.0000E+00	0.0000E+00	0.5350E+03	0.3315E+03	0.1530E+03	0.5000E+02	0.5000E+02	0.6100E+02	0.9250E+01	0.6950E+01	0.1820E+02

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: W 45.0 KV
GEOMETRY: 63,33 DEGREES

ANALYTE: CR (24)

		24 CR	26 FE	28 NI
	A1	0.000	-0.107	0.025
	A2	0.000	-0.334	-0.328
	A3	0.000	0.696	0.261
AIJK	24 CR	0.000		
	26 FE	0.000		
	28 NI	0.000	0.384	

ANALYTE: FE (26)

		24 CR	26 FE	28 NI
	A1	2.197	0.000	-0.179
	A2	-0.197	0.000	-0.297
	A3	-0.756	0.000	0.588
AIJK	24 CR	0.000		
	26 FE	0.000		
	28 NI	-0.291	0.000	

ANALYTE: NI (28)

		24 CR	26 FE	28 NI
	A1	1.314	1.834	0.000
	A2	-0.178	-0.218	0.000
	A3	-0.689	-0.745	0.000
AIJK	24 CR	0.000		
	26 FE	0.000		
	28 NI	0.000	0.000	

3.1B Calculated Compositions for Cr-Fe-Ni Alloys Using one Type Standard

```
$RUN CALCOMP


DATE:  02-OCT-84      TIME:  15:52:55

WHAT TYPE OF UNKNOWNS DO YOU WISH TO ANALYZE :
  1-ELEMENT SYSTEM    2-OXIDE SYSTEM    3-FUSED DISK SYSTEM  ?  1
DO YOU WANT TO INPUT KNOWN CONCENTRATIONS OF UNANALYZED ELEMENTS (Y/N)?  N
INPUT N(NUMBER OF ANALYTES) & M(NUMBER OF SPECIMENS TO BE ANALYZED) :  3,3
INPUT NAMES OF ANALYTES(XXXXXXXX)(MAX.=8/LINE) :

CR      FE      NI
DO YOU WANT TO INPUT ALPHA COEFFICIENTS BY: 1-DATAFILE  2-KEYBOARD  ?  2
TYPE IN THE ALPHA COEFFICIENTS :

0.0,-.107,.025,0.0,-.334,-.328,0.0,.696,.261,3*0.0,3*0.0,0.0,.384,0.0
2.197,0.0,-.179,-.197,0.0,-.297,-.756,0.0,.588,3*0.0,3*0.0,-.291,2*0.0
1.314,1.834,0.0,-.178,-.218,0.0,-.689,-.745,0.0,3*0.0,3*0.0,3*0.0
WHAT TYPE OF STANDARDS ARE AVAILABLE: 1-PURE STANDARDS    2-MULTIELEMENT STANDARDS  ?  2
INPUT M1(NUMBER OF STANDARDS) :  1
INPUT I.D. OF STANDARDS (<=8 CHARACTERS) :

 I= 1    5074
INPUT CONCENTRATIONS(WEIGHT FRACTION) OF STANDARDS :

 I= 1    5074      .2525,.6838,.0498
INPUT NET INTENSITIES FOLLOWED BY A PERIOD FOR THE ANALYTE ELEMENTS IN STANDARDS :
 I= 1    5074      3258.,4522.,203.
INPUT I.D. OF SPECIMENS TO BE ANALYZED :

 I= 1    5054
 I= 2    5202
 I= 3    5364
INPUT NET INTENSITIES OF SPECIMENS TO BE ANALYZED :

 I= 1    5054      3348.,4689.,6.
 I= 2    5202      2784.,4480.,642.
 I= 3    5364      3361.,3179.,1115.
DO YOU WANT TO CORRECT INTENSITIES FOR DEAD TIME (Y/N) ?  N
DO YOU WANT TO PRINT OUT CALCULATED RELATIVE INTENSITIES OF STANDARDS &
  CALCULATED PURE INTENSITIES FROM STANDARDS (Y/N) ?  Y

CALCULATED RELATIVE INTENSITIES OF STANDARDS :
                  CR       FE       NI
STD.NO.=5074      0.32018  0.45370  0.02079

CALCULATED PURE INTENSITIES FROM STANDARDS :
                  CR       FE       NI
STD.NO.=5074        10175.    9967.    9764.

AVERAGE VALUES      10175.    9967.    9764.

BECAUSE ONLY ONE STANDARD IS AVAILABLE, THE ONLY CHOICE FOR LSF CALIBRATION CURVE IS:  Y=A1*X.
DO YOU WANT TO PRINT OUT LSF COEFFICIENTS (Y/N) :  Y

            TABULATION OF CALCULATED LSF COEFFICIENTS
               (X=MEAS.INT.  ;  Y=CALC.REL.INT.)

CR        A0= 0.00000E+00  A1= 0.98276E-04  A2= 0.00000E+00
FE        A0= 0.00000E+00  A1= 0.10033E-03  A2= 0.00000E+00
NI        A0= 0.00000E+00  A1= 0.10242E-03  A2= 0.00000E+00

-----RESULTS OF LAST ITERATION-----
```

3.1B Calculated Compositions for Cr-Fe-Ni Alloys Using one Type Standard (Continued)

```
SMP.NO.=5054      R=CR      0.32903 FE      0.47045 NI      0.00061
          L= 6    C=CR     25.576% FE     72.067% NI       0.150%
                  TOTAL=  97.80%

SMP.NO.=5202      R=CR      0.27360 FE      0.44948 NI      0.06575
          L= 6    C=CR     21.744% FE     62.906% NI      14.938%
                  TOTAL=  99.59%

SMP.NO.=5364      R=CR      0.33031 FE      0.31895 NI      0.11419
          L= 6    C=CR     28.179% FE     47.279% NI      23.943%
                  TOTAL=  99.40%
```

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	CR	FE	NI
5054	97.80	25.576	72.067	0.150
5202	99.59	21.744	62.906	14.938
5364	99.40	28.179	47.279	23.943

```
DO YOU WISH TO COMPARE THESE RESULTS WITH OTHER PREVIOUSLY KNOWN VALUES FOR THESE SPECIMENS (Y/N) ?  Y
ENTER KNOWN CONCENTRATIONS OF SPECIMENS :

SMP.NO.=5054      .2577,.7250,.0015
SMP.NO.=5202      .2130,.6303,.1480
SMP.NO.=5364      .2784,.4721,.2357
```

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	CR	FE	NI
5054	98.42	25.77	72.50	0.15
	97.80	25.58	72.07	0.15
	ABS.ERR.	-0.19	-0.43	0.00
	REL.ERR.	-0.74	-0.59	0.00
5202	99.13	21.30	63.03	14.80
	99.59	21.74	62.91	14.94
	ABS.ERR.	0.44	-0.12	0.14
	REL.ERR.	2.07	-0.19	0.95
5364	98.62	27.84	47.21	23.57
	99.40	28.18	47.28	23.94
	ABS.ERR.	0.34	0.07	0.37
	REL.ERR.	1.22	0.15	1.57
	AVG.ABS.ERR.	0.32	0.21	0.17
	AVG.REL.ERR.	1.34	0.31	0.84

3.2A Calculation of Coefficients for High Temperature Alloys

```
$RUN CALCO


DATE:  02-OCT-84      TIME:  16:01:18

WHICH SYSTEM DO YOU WISH TO ANALYZE:
  1-ELEMENT SYSTEM  2-OXIDE SYSTEM  3-FUSED DISK SYSTEM  ?  1
INPUT NUMBER OF ANALYTES:  12
INPUT NAMES OF ANALYTES (XXS):  C  AL SI V  CR MN FE CO NI CU NB MO
WHAT MASS ABS. COEF. ALGORITHM DO YOU WANT TO USE :
  1-LEROUX ALGORITHM  2-HEINRICH ALGORITHM ?  2
DO YOU WANT TO CREATE A DATAFILE FOR SAVING CALCULATED ALPHA COEFFICIENTS (Y/N)?  Y
INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX) :  ALLOY2.C45
FOR SAMPLE GEOMETRY, INPUT INCIDENCE & EMERGENCE ANGLES (DEGREE-XX):  55,35
INPUT THE CHARACTERISTIC LINE NUMBER YOU WISH TO MEASURE (1-KA, 2-KB, 3-LA1, 4-LB1, 5-LB2):
I= 1    C     1
I= 2    AL    1
I= 3    SI    1
I= 4    V     1
I= 5    CR    1
I= 6    MN    1
I= 7    FE    1
I= 8    CO    1
I= 9    NI    1
I=10    CU    1
I=11    NB    1
I=12    MO    1
DO YOU WANT TO PRINT OUT CALCULATED ALPHA COEFFICIENTS(Y/N):  Y
WHICH X-RAY TUBE SPECTRAL DISTRIBUTION DO YOU PREFER:
  1-CALCULATED SPECTRUM FROM NBS ALGORITHM  ;  2-MEASURED SPECTRUM ?  1
DO YOU WANT TO PRINT OUT THE SPECTRAL DISTRIBUTION(Y/N) ?  Y
INPUT NAME OF X-RAY TUBE TARGET (XX) :  CR
INPUT VOLTAGE(KV), TAKE-OFF ANGLE OF X-RAY FROM TUBE TARGET(DEGREE), AND
   WINDOW THICKNESS(MM) OF X-RAY TUBE :  45.0,26.0,.45
INPUT THE ENDING WAVELENGTH OF X-RAY TUBE SPECTRUM(ANGSTROM) :  2.99
```

CALCULATED X-RAY TUBE SPECTRAL DISTRIBUTION
USING NBS ALGORITHM

X-RAY TUBE TARGET: CR KV: 45.0
TAKE-OFF ANGLE(DEGREE): 26.0 BE WINDOW THICKNESS(MM): 0.450

LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A
0.2755	0.0000E+00	0.2955	0.5418E-04	0.3155	0.9495E-04	0.3355	0.1258E-03	0.3555	0.1492E-03
0.3755	0.1669E-03	0.3955	0.1802E-03	0.4155	0.1900E-03	0.4355	0.1973E-03	0.4555	0.2024E-03
0.4755	0.2058E-03	0.4955	0.2078E-03	0.5155	0.2088E-03	0.5355	0.2089E-03	0.5555	0.2083E-03
0.5755	0.2072E-03	0.5955	0.2055E-03	0.6155	0.2035E-03	0.6355	0.2012E-03	0.6555	0.1986E-03
0.6755	0.1958E-03	0.6955	0.1929E-03	0.7155	0.1898E-03	0.7355	0.1866E-03	0.7555	0.1834E-03
0.7755	0.1801E-03	0.7955	0.1768E-03	0.8155	0.1734E-03	0.8355	0.1700E-03	0.8555	0.1666E-03
0.8755	0.1633E-03	0.8955	0.1599E-03	0.9155	0.1565E-03	0.9355	0.1532E-03	0.9555	0.1499E-03
0.9755	0.1466E-03	0.9955	0.1433E-03	1.0155	0.1401E-03	1.0355	0.1369E-03	1.0555	0.1338E-03
1.0755	0.1307E-03	1.0955	0.1276E-03	1.1155	0.1246E-03	1.1355	0.1216E-03	1.1555	0.1187E-03
1.1755	0.1158E-03	1.1955	0.1130E-03	1.2155	0.1102E-03	1.2355	0.1075E-03	1.2555	0.1048E-03
1.2755	0.1022E-03	1.2955	0.9958E-04	1.3155	0.9704E-04	1.3355	0.9455E-04	1.3555	0.9211E-04
1.3755	0.8972E-04	1.3955	0.8737E-04	1.4155	0.8508E-04	1.4355	0.8283E-04	1.4555	0.8063E-04
1.4755	0.7848E-04	1.4955	0.7638E-04	1.5155	0.7432E-04	1.5355	0.7231E-04	1.5555	0.7035E-04
1.5755	0.6843E-04	1.5955	0.6655E-04	1.6155	0.6473E-04	1.6355	0.6294E-04	1.6555	0.6120E-04
1.6755	0.5950E-04	1.6955	0.5784E-04	1.7155	0.5622E-04	1.7355	0.5465E-04	1.7555	0.5311E-04
1.7755	0.5161E-04	1.7955	0.5015E-04	1.8155	0.4873E-04	1.8355	0.4735E-04	1.8555	0.4600E-04
1.8755	0.4469E-04	1.8955	0.4342E-04	1.9155	0.4217E-04	1.9355	0.4097E-04	1.9555	0.3979E-04
1.9755	0.3865E-04	1.9955	0.3753E-04	2.0155	0.3645E-04	2.0355	0.3540E-04	2.0555	0.3438E-04
2.0755	0.6766E-04	2.0955	0.6643E-04	2.1155	0.6521E-04	2.1355	0.6401E-04	2.1555	0.6283E-04
2.1755	0.6166E-04	2.1955	0.6050E-04	2.2155	0.5937E-04	2.2355	0.5824E-04	2.2555	0.5713E-04
2.2755	0.5604E-04	2.2955	0.5496E-04	2.3155	0.5389E-04	2.3355	0.5284E-04	2.3555	0.5180E-04
2.3755	0.5077E-04	2.3955	0.4976E-04	2.4155	0.4877E-04	2.4355	0.4779E-04	2.4555	0.4682E-04
2.4755	0.4586E-04	2.4955	0.4492E-04	2.5155	0.4399E-04	2.5355	0.4308E-04	2.5555	0.4218E-04
2.5755	0.4129E-04	2.5955	0.4042E-04	2.6155	0.3955E-04	2.6355	0.3871E-04	2.6555	0.3787E-04
2.6755	0.3705E-04	2.6955	0.3624E-04	2.7155	0.3544E-04	2.7355	0.3465E-04	2.7555	0.3388E-04
2.7755	0.3312E-04	2.7955	0.3237E-04	2.8155	0.3164E-04	2.8355	0.3091E-04	2.8555	0.3020E-04
2.8755	0.2950E-04	2.8955	0.2881E-04	2.9155	0.2814E-04	2.9355	0.2747E-04	2.9555	0.2682E-04
2.9755	0.2618E-04								

KA	KB	LA1	LB1	LB2	LB3	LB4	LG1	LG2	LG3	LL
2.2910	2.0850	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.2353E-01	0.3627E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: C (6)

		6	13	14	23	24	25	26	27	28	29	41	42
		C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1	0.000	-2.089	-2.020	-2.733	-2.313	-2.273	-2.217	-2.154	-2.198	-2.133	-1.983	-1.969
	A2	0.000	1.565	1.620	2.106	1.746	1.759	1.762	1.762	1.758	1.754	1.578	1.573
	A3	0.000	-0.976	-0.967	-0.976	-0.987	-0.988	-0.989	-0.990	-0.991	-0.992	-0.998	-0.998
AIJK	6 C	0.000											
	13 AL	0.000											
	14 SI	0.000	0.335										
	23 V	0.000	0.192	0.259									
	24 CR	0.000	0.209	0.277	-0.025								
	25 MN	0.000	0.215	0.287	0.011	-0.002							
	26 FE	0.000	0.221	0.297	0.008	0.032	-0.002						
	27 CO	0.000	0.226	0.306	0.005	0.028	0.029	-0.002					
	28 NI	0.000	0.235	0.321	0.008	0.024	0.024	0.025	-0.001				
	29 CU	0.000	0.241	0.329	0.006	0.021	0.022	0.022	0.024	-0.002			
	41 NB	0.000	0.168	0.225	0.048	0.026	0.023	0.021	0.018	0.013	0.011		
	42 MO	0.000	0.176	0.236	0.051	0.027	0.024	0.022	0.019	0.014	0.012	-0.000	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: AL (13)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		0.184	0.000	0.229	4.400	5.163	6.005	6.918	7.903	8.963	10.098	3.821	4.184
	A2		-0.002	0.000	-0.281	-0.264	-0.142	-0.146	-0.147	-0.148	-0.145	-0.144	0.001	0.000
	A3		-0.203	0.000	4.309	-0.137	-0.122	-0.225	-0.314	-0.392	-0.462	-0.524	-1.063	-1.142
AIJK	6	C	0.000											
	13	AL	0.000											
	14	SI	-0.002	0.000										
	23	V	0.033	0.000	0.048									
	24	CR	0.027	0.000	-0.112	-0.133								
	25	MN	0.029	0.000	-0.136	0.026	-0.010							
	26	FE	0.029	0.000	-0.165	-0.009	0.175	-0.013						
	27	CO	0.029	0.000	-0.195	-0.047	0.156	0.175	-0.014					
	28	NI	0.028	0.000	-0.228	-0.090	0.132	0.151	0.173	-0.015				
	29	CU	0.026	0.000	-0.259	-0.132	0.109	0.127	0.150	0.173	-0.014			
	41	NB	-0.004	0.000	-0.215	0.270	0.151	0.158	0.160	0.160	0.156	0.152		
	42	MO	-0.003	0.000	-0.230	0.271	0.152	0.160	0.162	0.162	0.159	0.155	-0.001	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: SI (14)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		-0.166	6.934	0.000	2.896	3.422	4.024	4.678	5.383	6.143	6.957	2.706	2.984
	A2		-0.003	-0.028	0.000	-0.200	-0.108	-0.111	-0.112	-0.113	-0.112	-0.112	0.001	0.000
	A3		0.118	-0.881	0.000	-0.060	-0.053	-0.160	-0.254	-0.339	-0.417	-0.487	-1.075	-1.322
AIJK	6	C	0.000											
	13	AL	0.001											
	14	SI	0.000	0.000										
	23	V	0.031	-0.255	0.000									
	24	CR	0.022	-0.093	0.000	-0.087								
	25	MN	0.023	-0.089	0.000	0.024	-0.007							
	26	FE	0.023	-0.082	0.000	-0.001	0.122	-0.009						
	27	CO	0.023	-0.075	0.000	-0.028	0.108	0.122	-0.010					
	28	NI	0.023	-0.067	0.000	-0.058	0.091	0.105	0.121	-0.010				
	29	CU	0.022	-0.060	0.000	-0.088	0.075	0.088	0.104	0.121	-0.010			
	41	NB	-0.002	-0.015	0.000	0.183	0.102	0.107	0.108	0.109	0.107	0.106		
	42	MO	-0.002	-0.012	0.000	0.184	0.102	0.107	0.109	0.110	0.109	0.107	-0.001	

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: V (23)

		6	13	14	23	24	25	26	27	28	29	41	42
		C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1	-0.917	-0.156	0.037	0.000	-0.277	-0.349	-0.301	-0.248	-0.186	-0.116	1.459	1.621
	A2	-0.011	-0.115	-0.142	0.000	-0.209	-0.195	-0.191	-0.184	-0.179	-0.175	-0.328	-0.349
	A3	9.635	-0.132	-0.292	0.000	0.344	0.156	0.004	-0.109	-0.194	-0.258	-0.688	-0.708
AIJK	6 C	0.000											
	13 AL	0.031											
	14 SI	0.037	0.000										
	23 V	0.000	0.000	0.000									
	24 CR	0.084	0.065	0.067	0.000								
	25 MN	0.064	-0.011	-0.020	0.000	-0.006							
	26 FE	0.058	-0.022	-0.032	0.000	0.140	0.008						
	27 CO	0.051	-0.031	-0.041	0.000	0.147	0.133	0.004					
	28 NI	0.046	-0.035	-0.045	0.000	0.148	0.127	0.124	0.001				
	29 CU	0.043	-0.037	-0.046	0.000	0.146	0.118	0.115	0.116	-0.002			
	41 NB	0.061	0.000	-0.004	0.000	0.100	-0.038	-0.051	-0.057	-0.056	-0.053		
	42 MO	0.063	0.002	-0.003	0.000	0.100	-0.045	-0.058	-0.064	-0.063	-0.060	-0.002	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: CR (24)

		6	13	14	23	24	25	26	27	28	29	41	42
		C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1	-0.874	0.282	0.577	-0.120	0.000	0.130	-0.070	0.016	0.111	0.206	2.486	2.746
	A2	-0.005	-0.047	-0.058	-0.000	0.000	-0.000	-0.421	-0.449	-0.474	-0.496	-0.524	-0.513
	A3	7.365	-0.063	-0.229	-0.924	0.000	-0.523	0.871	0.615	0.422	0.266	-0.317	-0.363
AIJK	6 C	0.000											
	13 AL	0.013											
	14 SI	0.016	0.000										
	23 V	0.002	0.046	0.055									
	24 CR	0.000	0.000	0.000	0.000								
	25 MN	0.002	0.046	0.056	0.000	0.000							
	26 FE	0.146	-0.242	-0.323	0.386	0.000	-0.279						
	27 CO	0.153	-0.276	-0.367	0.420	0.000	0.432	0.000					
	28 NI	0.159	-0.302	-0.401	0.448	0.000	0.462	0.591	0.000				
	29 CU	0.161	-0.331	-0.437	0.469	0.000	0.484	0.626	0.645	-0.000			
	41 NB	0.166	-0.083	-0.136	0.453	0.000	0.482	-0.016	-0.064	-0.097	-0.133		
	42 MO	0.159	-0.070	-0.119	0.436	0.000	0.465	-0.102	-0.157	-0.198	-0.240	-0.035	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: MN (25)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		-0.894	0.081	0.330	3.994	-0.114	0.000	0.122	-0.114	-0.034	0.046	1.927	2.151
	A2		-0.005	-0.048	-0.059	-0.220	-0.000	0.000	-0.001	-0.399	-0.420	-0.438	-0.445	-0.438
	A3		7.654	0.123	-0.085	-0.752	-0.931	0.000	697.862	0.768	0.549	0.368	-0.273	-0.327
AIJK	6	C	0.000											
	13	AL	0.014											
	14	SI	0.018	0.000										
	23	V	0.039	0.009	0.006									
	24	CR	0.002	0.047	0.057	0.132								
	25	MN	0.000	0.000	0.000	0.000	0.000							
	26	FE	0.002	0.047	0.058	0.139	0.001	0.000						
	27	CO	0.142	-0.199	-0.271	-1.006	0.370	0.000	-0.310					
	28	NI	0.148	-0.221	-0.300	-1.107	0.396	0.000	0.406	0.001				
	29	CU	0.150	-0.247	-0.332	-1.212	0.415	0.000	0.427	0.571	0.001			
	41	NB	0.144	-0.071	-0.115	-0.591	0.389	0.000	0.411	-0.017	-0.045	-0.075		
	[illegible]	MO	0.139	-0.059	-0.100	-0.537	0.378	0.000	0.400	-0.094	-0.128	-0.164	-0.030	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: FE (26)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		-0.932	-0.300	-0.139	2.248	2.619	-0.105	0.000	0.044	-0.224	-0.191	1.006	1.150
	A2		-0.007	-0.073	-0.089	-0.336	-0.374	0.000	0.000	-0.118	-0.294	-0.280	-0.230	-0.242
	A3		15.515	0.388	0.140	-0.689	-0.720	-1.156	0.000	1.459	0.496	0.288	-0.442	-0.485
AIJK	6	C	0.000											
	13	AL	0.023											
	14	SI	0.029	0.000										
	23	V	0.072	0.018	0.014									
	24	CR	0.075	0.020	0.016	0.000								
	25	MN	0.002	0.071	0.088	0.228	0.240							
	26	FE	0.000	0.000	0.000	0.000	0.000	0.000						
	27	CO	0.052	0.083	0.093	0.188	0.196	0.103	0.000					
	28	NI	0.112	-0.031	-0.057	-0.321	-0.350	0.276	0.000	-0.178				
	29	CU	0.101	-0.051	-0.079	-0.353	-0.383	0.263	0.000	0.281	0.009			
	41	NB	0.064	-0.010	-0.019	-0.088	-0.095	0.194	0.000	0.187	-0.094	-0.112		
	42	MO	0.065	-0.007	-0.016	-0.080	-0.086	0.199	0.000	0.188	-0.120	-0.139	-0.007	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: CO (27)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		-0.941	-0.386	-0.243	1.863	2.192	2.539	-0.100	0.000	0.038	-0.253	0.753	0.881
	A2		-0.006	-0.061	-0.075	-0.282	-0.314	-0.348	-0.000	0.000	-0.116	-0.280	-0.197	-0.205
	A3		18.054	0.542	0.273	-0.654	-0.689	-0.719	2.416	0.000	1.422	0.464	-0.372	-0.419
AIJK	6	C	0.000											
	13	AL	0.020											
	14	SI	0.025	0.000										
	23	V	0.066	0.018	0.013									
	24	CR	0.069	0.020	0.015	0.000								
	25	MN	0.072	0.022	0.017	0.000	0.000							
	26	FE	0.002	0.059	0.073	0.202	0.214	0.224						
	27	CO	0.000	0.000	0.000	0.000	0.000	0.000	0.000					
	28	NI	0.052	0.076	0.085	0.172	0.180	0.188	0.101	0.000				
	29	CU	0.108	-0.030	-0.056	-0.324	-0.353	-0.383	0.263	0.000	-0.200			
	41	NB	0.058	-0.012	-0.022	-0.095	-0.103	-0.110	0.171	0.000	0.174	-0.079		
	42	MO	0.059	-0.009	-0.018	-0.086	-0.093	-0.099	0.175	0.000	0.175	-0.106	[illegible]	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: NI (28)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		-0.948	-0.458	-0.332	1.536	1.828	2.137	2.463	-0.096	0.000	0.036	0.538	0.653
	A2		-0.005	-0.051	-0.063	-0.238	-0.266	-0.294	-0.325	-0.000	0.000	-0.111	-0.171	-0.177
	A3		19.257	0.716	0.414	-0.616	-0.655	-0.688	-0.717	-0.944	0.000	1.409	-0.296	-0.348
AIJK	6	C	0.000											
	13	AL	0.017											
	14	SI	0.022	0.000										
	23	V	0.060	0.017	0.013									
	24	CR	0.063	0.019	0.015	0.000								
	25	MN	0.066	0.021	0.016	0.000	0.000							
	26	FE	0.069	0.023	0.018	0.001	0.000	0.000						
	27	CO	0.001	0.049	0.061	0.180	0.191	0.201	0.210					
	28	NI	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000				
	29	CU	0.050	0.070	0.078	0.160	0.168	0.176	0.183	0.096	0.000			
	41	NB	0.053	-0.014	-0.024	-0.104	-0.112	-0.119	-0.127	0.151	0.000	0.164		
	42	MO	0.054	-0.011	-0.020	-0.094	-0.101	-0.108	-0.115	0.155	0.000	0.165	-0.008	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: CU (29)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		-0.954	-0.520	-0.409	1.253	1.513	1.788	2.079	2.384	-0.092	0.000	0.352	0.455
	A2		-0.004	-0.044	-0.054	-0.204	-0.227	-0.252	-0.278	-0.306	-0.000	0.000	-0.151	-0.155
	A3		19.672	0.909	0.566	-0.573	-0.617	-0.654	-0.686	-0.714	-0.862	0.000	-0.221	-0.274
AIJK	6	C	0.000											
	13	AL	0.015											
	14	SI	0.019	0.000										
	23	V	0.056	0.016	0.013									
	24	CR	0.058	0.018	0.014	0.000								
	25	MN	0.061	0.020	0.016	0.000	0.000							
	26	FE	0.064	0.022	0.018	0.001	0.000	0.000						
	27	CO	0.066	0.024	0.019	0.001	0.000	0.000	0.000					
	28	NI	0.001	0.040	0.052	0.161	0.172	0.182	0.191	0.199				
	29	CU	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
	41	NB	0.048	-0.017	-0.027	-0.112	-0.120	-0.129	-0.137	-0.145	0.136	0.000		
	42	MO	0.049	-0.013	-0.023	-0.101	-0.109	-0.117	-0.124	-0.132	0.138	0.000	-0.008	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: NB (41)

			6	13	14	23	24	25	26	27	28	29	41	42
			C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1		-0.986	-0.846	-0.809	-0.249	-0.160	-0.066	0.035	0.141	0.252	0.370	0.000	0.011
	A2		-0.001	-0.006	-0.007	-0.029	-0.032	-0.035	-0.039	-0.043	-0.047	-0.052	0.000	-0.076
	A3		8.760	5.483	3.296	0.200	0.081	-0.028	-0.116	-0.198	-0.268	-0.334	0.000	1.239
AIJK	6	C	0.000											
	13	AL	0.002											
	14	SI	0.002	0.000										
	23	V	0.012	0.006	0.005									
	24	CR	0.014	0.006	0.005	0.000								
	25	MN	0.015	0.007	0.006	0.000	0.000							
	26	FE	0.016	0.008	0.007	0.000	0.000	0.000						
	27	CO	0.017	0.009	0.008	0.001	0.000	0.000	0.000					
	28	NI	0.019	0.010	0.009	0.001	0.000	0.000	0.000	0.000				
	29	CU	0.020	0.011	0.010	0.001	0.001	0.000	0.000	0.000	0.000			
	41	NB	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
	42	MO	0.036	0.038	0.038	0.057	0.059	0.062	0.065	0.068	0.071	0.074	0.000	

BASIC ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(ELEMENTAL SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: MO (42)

		6	13	14	23	24	25	26	27	28	29	41	42
		C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
	A1	-0.987	-0.860	-0.827	-0.316	-0.235	-0.149	-0.057	0.040	0.142	0.249	-0.062	0.000
	A2	-0.000	-0.005	-0.006	-0.025	-0.028	-0.031	-0.034	-0.038	-0.041	-0.045	0.000	0.000
	A3	-4.860	5.793	4.410	0.322	0.187	0.073	-0.032	-0.120	-0.197	-0.263	-1.028	0.000
AIJK	6 C	0.000											
	13 AL	0.001											
	14 SI	0.002	0.000										
	23 V	0.011	0.005	0.004									
	24 CR	0.012	0.006	0.005	0.000								
	25 MN	0.013	0.007	0.006	0.000	0.000							
	26 FE	0.015	0.008	0.007	0.000	0.000	0.000						
	27 CO	0.016	0.009	0.007	0.001	0.000	0.000	0.000					
	28 NI	0.017	0.009	0.008	0.001	0.000	0.000	0.000	0.000				
	29 CU	0.018	0.010	0.009	0.001	0.001	0.000	0.000	0.000	0.000			
	41 NB	0.000	0.003	0.004	0.025	0.028	0.031	0.034	0.037	0.040	0.043		
	42 MO	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	

3.2B Calculated Compositions of High Temperature Alloys. (Six Analytes Plus Known Concentrations of Minor Elements)

```
$RUN CALCOMP


DATE:  03-OCT-84      TIME:  08:19:00

WHAT TYPE OF UNKNOWNS DO YOU WISH TO ANALYZE :
  1-ELEMENT SYSTEM    2-OXIDE SYSTEM    3-FUSED DISK SYSTEM  ?  1
DO YOU WANT TO INPUT KNOWN CONCENTRATIONS OF UNANALYZED ELEMENTS (Y/N)?  Y
INPUT N6(NUMBER OF ALL CONSTITUENTS), N(NUMBER OF ANALYTES) AND
  M(NUMBER OF SPECIMENS TO BE ANALYZED) :          12,6,4
INPUT NAMES OF CONSTITUENTS(XXXXXXXX)(MAX.=8/LINE) :

C       AL      SI      V       CR      MN      FE      CO
NI      CU      NB      MO
INPUT NAMES OF ANALYTES(XXXXXXXX)(MAX.=8/LINE) :

CR      MN      FE      NI      CU      MO
DO YOU WANT TO INPUT ALPHA COEFFICIENTS BY: 1-DATAFILE  2-KEYBOARD  ?  1
INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX) :  ALLOY2.C45
WHAT TYPE OF STANDARDS ARE AVAILABLE: 1-PURE STANDARDS    2-MULTIELEMENT STANDARDS  ?  2
INPUT M1(NUMBER OF STANDARDS) :  5
INPUT I.D. OF STANDARDS (<=8 CHARACTERS) :

 I= 1    C1151
 I= 2    C1153
 I= 3    C1285
 I= 4    C1288
 I= 5    C1289
INPUT CONCENTRATIONS(WEIGHT FRACTION) OF STANDARDS :

 I= 1    C1151     .0004,0.0,.0038,.0004,.2270,.0250,.6536,.0003,.0729,.0042,0.0,.0080
 I= 2    C1153     .0026,0.0,.0107,.0018,.1669,.0050,.7096,.0013,.0377,.0023,0.0,.0024
 I= 3    C1285     .0006,.0012,.0036,.0015,.0080,.0033,.9633,.0004,.0117,.0037,0.0,.0016
 I= 4    C1288     .0006,0.0,.0041,.0009,.1955,.0083,.4155,.0010,.2930,.0372,.0022,.0283
 I= 5    C1289     .0001,0.0,.0016,.0001,.1222,.0035,.8172,.0004,.0413,.0021,.0010,.0082
INPUT NET INTENSITIES FOLLOWED BY A PERIOD FOR THE ANALYTE ELEMENTS IN STANDARDS AND
  ENTER 0.0 FOR EACH UNANALYZED ELEMENT:

 I= 1    C1151     4*0.0,16511.,141.,11810.,0.0,2892.,211.,0.0,1248.
 I= 2    C1153     4*0.0,13016.,29.,14027.,0.0,3486.,119.,0.0,294.
 I= 3    C1285     4*0.0,917.,19.,24913.,0.0,417.,163.,0.0,239.
 I= 4    C1288     4*0.0,12598.,46.,8736.,0.0,14190.,2211.,0.0,4016.
 I= 5    C1289     4*0.0,10265.,19.,17093.,0.0,1552.,102.,0.0,1220.
INPUT I.D. OF SPECIMENS TO BE ANALYZED :

 I= 1    C1152
 I= 2    C1154
 I= 3    1286
 I= 4    C1287
INPUT NET INTENSITIES FOR ANALYTES IN SPECIMENS AND
  ENTER CONCENTRATIONS(WEIGHT FRACTION) FOR UNANALYZED ELEMENTS:

 I= 1    C1152     .0015,0.0,.0080,.0003,13579.,54.,13316.,.0022,4367.,60.,0.0,640.
 I= 2    C1154     .0009,0.0,.0050,.0014,14272.,82.,12448.,.0038,5250.,207.,0.0,78.
 I= 3    1286      .0020,.0011,.0013,.0001,1659.,8.,24071.,.0012,1014.,23.,.0001,504.
 I= 4    C1287     .0036,.0006,.0166,.0009,16245.,87.,9578.,.0031,9088.,329.,.0007,723.
DO YOU WANT TO CORRECT INTENSITIES FOR DEAD TIME (Y/N) ?  N
DO YOU WANT TO PRINT OUT CALCULATED RELATIVE INTENSITIES OF STANDARDS &
  CALCULATED PURE INTENSITIES FROM STANDARDS (Y/N) ?  Y

CALCULATED RELATIVE INTENSITIES OF STANDARDS :
                  CR        MN        FE        NI        CU        MO
STD.NO.=C1151     0.28026   0.02344   0.43075   0.02597   0.00167   0.00908
```

```
STD.NO.=C1153      0.22000  0.00467  0.51727  0.03140  0.00092  0.00270
STD.NO.=C1285      0.01477  0.00293  0.94394  0.00380  0.00134  0.00177
STD.NO.=C1288      0.21031  0.00807  0.31037  0.13036  0.01832  0.03000
STD.NO.=C1289      0.17454  0.00317  0.63051  0.01399  0.00080  0.00915

CALCULATED PURE INTENSITIES FROM STANDARDS :
                     CR       MN       FE       NI       CU       MO
STD.NO.=C1151       58913.    6017.   27417.  111375.  126289.  137479.
STD.NO.=C1153       59164.    6215.   27117.  111027.  129615.  108819.
STD.NO.=C1285       62069.    6481.   26393.  109775.  121197.  135404.
STD.NO.=C1288       59903.    5697.   28147.  108854.  120670.  133866.
STD.NO.=C1289       58813.    5984.   27110.  110922.  128201.  133348.

AVERAGE VALUES      59772.    6079.   27237.  110391.  125194.  129783.

WHAT TYPE OF LSF CURVES DO YOU WANT TO USE FOR CALIBRATION :
  (1) Y=A0+A1*X      (2) Y=A0+A1*X+A2*X*X
  (3) Y=A1*X         (4) Y=A1*X+A2*X*X       ?  4
DO YOU WANT TO PRINT OUT LSF COEFFICIENTS (Y/N) :  Y

              TABULATION OF CALCULATED LSF COEFFICIENTS
                 (X=MEAS.INT.  ;  Y=CALC.REL.INT.)

CR        A0= 0.00000E+00  A1= 0.16663E-04  A2= 0.16886E-10
MN        A0= 0.00000E+00  A1= 0.16926E-03  A2=-0.20617E-07
FE        A0= 0.00000E+00  A1= 0.34960E-04  A2= 0.11799E-09
NI        A0= 0.00000E+00  A1= 0.89478E-05  A2= 0.16819E-10
CU        A0= 0.00000E+00  A1= 0.79401E-05  A2= 0.15693E-09
MO        A0= 0.00000E+00  A1= 0.74415E-05  A2= 0.63349E-11

-----RESULTS OF LAST ITERATION-----

SMP.NO.=C1152     R=CR      0.22939 MN      0.00908 FE      0.48645 NI      0.03940 CU      0.00048 MO      0.00477

          L= 7  C=C        0.150% AL       0.000% SI       0.800% V        0.030% CR      17.915% MN       0.963%
                FE        67.649% CO       0.220% NI      10.845% CU       0.116% NB       0.000% MO       0.427%

                TOTAL=  99.12%

SMP.NO.=C1154     R=CR      0.24126 MN      0.01374 FE      0.45347 NI      0.04744 CU      0.00165 MO      0.00058

          L= 7  C=C        0.090% AL       0.000% SI       0.500% V        0.140% CR      19.154% MN       1.438%
                FE        63.819% CO       0.380% NI      12.823% CU       0.403% NB       0.000% MO       0.051%

                TOTAL=  98.79%

SMP.NO.=1286      R=CR      0.02769 MN      0.00135 FE      0.90990 NI      0.00909 CU      0.00018 MO      0.00375

          L= 4  C=C        0.200% AL       0.110% SI       0.130% V        0.010% CR       1.561% MN       0.151%
                FE        94.158% CO       0.120% NI       2.766% CU       0.050% NB       0.010% MO       0.341%

                TOTAL=  99.61%

SMP.NO.=C1287     R=CR      0.27515 MN      0.01457 FE      0.34568 NI      0.08271 CU      0.00263 MO      0.00538

          L= 6  C=C        0.360% AL       0.060% SI       1.660% V        0.090% CR      23.730% MN       1.484%
                FE        50.591% CO       0.310% NI      20.605% CU       0.592% NB       0.070% MO       0.483%

                TOTAL= 100.02%
```

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
C1152	99.12	0.150	0.000	0.800	0.030	17.915	0.963	67.649	0.220	10.845	0.116	0.000	0.427
C1154	98.79	0.090	0.000	0.500	0.140	19.154	1.438	63.819	0.380	12.823	0.403	0.000	0.051
1286	99.61	0.200	0.110	0.130	0.010	1.561	0.151	94.158	0.120	2.766	0.050	0.010	0.341
C1287	100.02	0.360	0.060	1.660	0.090	23.730	1.484	50.591	0.310	20.605	0.592	0.070	0.483

DO YOU WISH TO COMPARE THESE RESULTS WITH OTHER PREVIOUSLY KNOWN VALUES FOR THESE SPECIMENS (Y/N) ? Y
ENTER KNOWN CONCENTRATIONS OF SPECIMENS :

SMP.NO.=C1152 .0015,0.0,.0080,.0003,.1781,.0096,.6797,.0022,.1088,.0010,0.0,.0043
SMP.NO.=C1154 .0009,0.0,.0050,.0014,.1906,.0142,.6442,.0038,.1292,.0040,0.0,.0007
SMP.NO.=1286 .0020,.0011,.0013,.0001,.0153,.0015,.9300,.0012,.0281,.0004,.0001,.0034
SMP.NO.=C1287 .0036,.0006,.0166,.0009,.2398,.0166,.4969,.0031,.2116,.0058,.0007,.0046

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	C	AL	SI	V	CR	MN	FE	CO	NI	CU	NB	MO
C1152	99.35	0.15	0.00	0.80	0.03	17.81	0.96	67.97	0.22	10.88	0.10	0.00	0.43
	99.12	0.15	0.00	0.80	0.03	17.91	0.96	67.65	0.22	10.85	0.12	0.00	0.43
	ABS.ERR.	0.00	0.00	0.00	0.00	0.10	0.00	-0.32	0.00	-0.03	0.02	0.00	0.00
	REL.ERR.	0.00	0.00	0.00	0.00	0.56	0.00	-0.47	0.00	-0.28	20.00	0.00	0.00
C1154	99.40	0.09	0.00	0.50	0.14	19.06	1.42	64.42	0.38	12.92	0.40	0.00	0.07
	98.79	0.09	0.00	0.50	0.14	19.15	1.44	63.82	0.38	12.82	0.40	0.00	0.05
	ABS.ERR.	0.00	0.00	0.00	0.00	0.09	0.02	-0.60	0.00	-0.10	0.00	0.00	-0.02
	REL.ERR.	0.00	0.00	0.00	0.00	0.47	1.41	-0.93	0.00	-0.77	0.00	0.00	-28.57
1286	98.45	0.20	0.11	0.13	0.01	1.53	0.15	93.00	0.12	2.81	0.04	0.01	0.34
	99.61	0.20	0.11	0.13	0.01	1.56	0.15	94.16	0.12	2.77	0.05	0.01	0.34
	ABS.ERR.	0.00	0.00	0.00	0.00	0.03	0.00	1.16	0.00	-0.04	0.01	0.00	0.00
	REL.ERR.	0.00	0.00	0.00	0.00	1.96	0.00	1.25	0.00	-1.42	25.00	0.00	0.00
C1287	100.08	0.36	0.06	1.66	0.09	23.98	1.66	49.69	0.31	21.16	0.58	0.07	0.46
	100.02	0.36	0.06	1.66	0.09	23.73	1.48	50.59	0.31	20.60	0.59	0.07	0.48
	ABS.ERR.	0.00	0.00	0.00	0.00	-0.25	-0.18	0.90	0.00	-0.56	0.01	0.00	0.02
	REL.ERR.	0.00	0.00	0.00	0.00	-1.04	-10.84	1.81	0.00	-2.65	1.72	0.00	4.35
	AVG.ABS.ERR.	0.00	0.00	0.00	0.00	0.12	0.05	0.75	0.00	0.18	0.01	0.00	0.01
	AVG.REL.ERR.	0.00	0.00	0.00	0.00	1.01	3.06	1.12	0.00	1.28	11.68	0.00	8.23

DO YOU WANT TO TRY ANOTHER TYPE OF CALIBRATION CURVE (Y/N) ? N

TTO — STOP

3.3A Calculation of Coefficients for Cement Samples as an Example of an Oxide System

```
$RUN CALCO


DATE:  03-OCT-84      TIME:  14:12:05

WHICH SYSTEM DO YOU WISH TO ANALYZE:
  1-ELEMENT SYSTEM  2-OXIDE SYSTEM  3-FUSED DISK SYSTEM  ?  2
INPUT NUMBER OF ANALYTES:  12
INPUT NAMES OF ANALYTES (XXNONS):

C 103 NA201 MG101 AL203 SI102 P 205 S 103 K 201 CA101 TI102 MN203 FE203
WHAT MASS ABS. COEF. ALGORITHM DO YOU WANT TO USE :
  1-LEROUX ALGORITHM  2-HEINRICH ALGORITHM ?  2
DO YOU WANT TO CREATE A DATAFILE FOR SAVING CALCULATED ALPHA COEFFICIENTS (Y/N)?  Y
INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX) :  OXCEMT.C45
FOR SAMPLE GEOMETRY, INPUT INCIDENCE & EMERGENCE ANGLES (DEGREE-XX):  55,35
INPUT THE CHARACTERISTIC LINE NUMBER YOU WISH TO MEASURE (1-KA, 2-KB, 3-LA1, 4-LB1, 5-LB2):
I= 1    C     1
I= 2    NA    1
I= 3    MG    1
I= 4    AL    1
I= 5    SI    1
I= 6    P     1
I= 7    S     1
I= 8    K     1
I= 9    CA    1
I=10    TI    1
I=11    MN    1
I=12    FE    1
DO YOU WANT TO PRINT OUT CALCULATED ALPHA COEFFICIENTS(Y/N):  Y
WHICH X-RAY TUBE SPECTRAL DISTRIBUTION DO YOU PREFER:
  1-CALCULATED SPECTRUM FROM NBS ALGORITHM  ;  2-MEASURED SPECTRUM ?  1
DO YOU WANT TO PRINT OUT THE SPECTRAL DISTRIBUTION(Y/N) ?  Y
INPUT NAME OF X-RAY TUBE TARGET (XX) :  CR
INPUT VOLTAGE(KV), TAKE-OFF ANGLE OF X-RAY FROM TUBE TARGET(DEGREE), AND
   WINDOW THICKNESS(MM) OF X-RAY TUBE :  45.0,26.0,.45
INPUT THE ENDING WAVELENGTH OF X-RAY TUBE SPECTRUM(ANGSTROM) :  2.9956
```

CALCULATED X-RAY TUBE SPECTRAL DISTRIBUTION
USING NBS ALGORITHM

X-RAY TUBE TARGET: CR KV: 45.0
TAKE-OFF ANGLE(DEGREE): 26.0 BE WINDOW THICKNESS(MM): 0.450

LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A
0.2755	0.0000E+00	0.2955	0.5418E-04	0.3155	0.9495E-04	0.3355	0.1258E-03	0.3555	0.1492E-03
0.3755	0.1669E-03	0.3955	0.1802E-03	0.4155	0.1900E-03	0.4355	0.1973E-03	0.4555	0.2024E-03
0.4755	0.2058E-03	0.4955	0.2078E-03	0.5155	0.2088E-03	0.5355	0.2089E-03	0.5555	0.2083E-03
0.5755	0.2072E-03	0.5955	0.2055E-03	0.6155	0.2035E-03	0.6355	0.2012E-03	0.6555	0.1986E-03
0.6755	0.1958E-03	0.6955	0.1929E-03	0.7155	0.1898E-03	0.7355	0.1866E-03	0.7555	0.1834E-03
0.7755	0.1801E-03	0.7955	0.1768E-03	0.8155	0.1734E-03	0.8355	0.1700E-03	0.8555	0.1666E-03
0.8755	0.1633E-03	0.8955	0.1599E-03	0.9155	0.1565E-03	0.9355	0.1532E-03	0.9555	0.1499E-03
0.9755	0.1466E-03	0.9955	0.1433E-03	1.0155	0.1401E-03	1.0355	0.1369E-03	1.0555	0.1338E-03
1.0755	0.1307E-03	1.0955	0.1276E-03	1.1155	0.1246E-03	1.1355	0.1216E-03	1.1555	0.1187E-03
1.1755	0.1158E-03	1.1955	0.1130E-03	1.2155	0.1102E-03	1.2355	0.1075E-03	1.2555	0.1048E-03
1.2755	0.1022E-03	1.2955	0.9958E-04	1.3155	0.9704E-04	1.3355	0.9455E-04	1.3555	0.9211E-04
1.3755	0.8972E-04	1.3955	0.8737E-04	1.4155	0.8508E-04	1.4355	0.8283E-04	1.4555	0.8063E-04
1.4755	0.7848E-04	1.4955	0.7638E-04	1.5155	0.7432E-04	1.5355	0.7231E-04	1.5555	0.7035E-04
1.5755	0.6843E-04	1.5955	0.6655E-04	1.6155	0.6473E-04	1.6355	0.6294E-04	1.6555	0.6120E-04
1.6755	0.5950E-04	1.6955	0.5784E-04	1.7155	0.5622E-04	1.7355	0.5465E-04	1.7555	0.5311E-04
1.7755	0.5161E-04	1.7955	0.5015E-04	1.8155	0.4873E-04	1.8355	0.4735E-04	1.8555	0.4600E-04
1.8755	0.4469E-04	1.8955	0.4342E-04	1.9155	0.4217E-04	1.9355	0.4097E-04	1.9555	0.3979E-04
1.9755	0.3865E-04	1.9955	0.3753E-04	2.0155	0.3645E-04	2.0355	0.3540E-04	2.0555	0.3438E-04
2.0755	0.6766E-04	2.0955	0.6643E-04	2.1155	0.6521E-04	2.1355	0.6401E-04	2.1555	0.6283E-04
2.1755	0.6166E-04	2.1955	0.6050E-04	2.2155	0.5937E-04	2.2355	0.5824E-04	2.2555	0.5713E-04
2.2755	0.5604E-04	2.2955	0.5496E-04	2.3155	0.5389E-04	2.3355	0.5284E-04	2.3555	0.5180E-04
2.3755	0.5077E-04	2.3955	0.4976E-04	2.4155	0.4877E-04	2.4355	0.4779E-04	2.4555	0.4682E-04
2.4755	0.4586E-04	2.4955	0.4492E-04	2.5155	0.4399E-04	2.5355	0.4308E-04	2.5555	0.4218E-04
2.5755	0.4129E-04	2.5955	0.4042E-04	2.6155	0.3955E-04	2.6355	0.3871E-04	2.6555	0.3787E-04
2.6755	0.3705E-04	2.6955	0.3624E-04	2.7155	0.3544E-04	2.7355	0.3465E-04	2.7555	0.3388E-04
2.7755	0.3312E-04	2.7955	0.3237E-04	2.8155	0.3164E-04	2.8355	0.3091E-04	2.8555	0.3020E-04
2.8755	0.2950E-04	2.8955	0.2881E-04	2.9155	0.2814E-04	2.9355	0.2747E-04	2.9555	0.2682E-04
2.9755	0.2618E-04	2.9955	0.2555E-04						

KA	KB	LA1	LB1	LB2	LB3	LB4	LG1	LG2	LG3	LL
2.2910	2.0850	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.2353E-01	0.3627E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: C 103 (6)

		6	11	12	13	14	15	16	19	20	22	25	26
		C 103	NA201	MG101	AL203	SI102	P 205	S 103	K 201	CA101	TI102	MN203	FE203
	A1	0.000	-0.090	0.039	0.202	0.358	0.567	0.756	2.161	-0.721	-0.668	0.273	0.425
	A2	0.000	-0.014	-0.012	-0.018	-0.026	-0.041	-0.054	-0.187	0.395	0.447	0.048	0.046
AIJK	6 C 103	0.000											
	11 NA201	0.000											
	12 MG101	0.000	0.061										
	13 AL203	0.000	0.081	0.078									
	14 SI102	0.000	0.106	0.103	0.105								
	15 P 205	0.000	0.147	0.144	0.145	0.147							
	16 S 103	0.000	0.188	0.185	0.187	0.188	0.196						
	19 K 201	0.000	0.657	0.669	0.686	0.697	0.719	0.737					
	20 CA101	0.000	-0.063	-0.067	-0.060	-0.048	-0.020	0.013	0.744				
	22 TI102	0.000	-0.107	-0.113	-0.108	-0.098	-0.071	-0.040	0.717	0.290			
	25 MN203	0.000	0.034	0.038	0.054	0.074	0.111	0.147	0.594	-0.159	-0.205		
	26 FE203	0.000	0.035	0.039	0.056	0.077	0.115	0.153	0.623	-0.169	-0.218	-0.003	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: NA2O1 (11)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 1O3	NA2O1	MGlO1	AL2O3	SIlO2	P 2O5	S 1O3	K 2O1	CAlO1	TIlO2	MN2O3	FE2O3
		A1	1.297	0.000	0.378	0.619	0.828	0.980	1.137	1.427	1.727	2.254	4.101	4.681
		A2	-0.000	0.000	-0.051	-0.071	-0.094	-0.124	-0.154	-0.333	-0.348	-0.345	-0.066	-0.064
AIJK	6	C 1O3	0.000											
	11	NA2O1	0.000											
	12	MGlO1	-0.015	0.000										
	13	AL2O3	-0.016	0.000	0.061									
	14	SIlO2	-0.017	0.000	0.081	0.082								
	15	P 2O5	-0.023	0.000	0.107	0.109	0.111							
	16	S 1O3	-0.029	0.000	0.134	0.135	0.138	0.145						
	19	K 2O1	-0.305	0.000	0.280	0.277	0.280	0.310	0.335					
	20	CAlO1	-0.315	0.000	0.288	0.285	0.287	0.317	0.341	0.727				
	22	TIlO2	-0.351	0.000	0.272	0.267	0.268	0.297	0.319	0.716	0.714			
	25	MN2O3	-0.019	0.000	0.020	0.013	0.006	-0.006	-0.022	-0.467	-0.493	-0.557		
	26	FE2O3	-0.017	0.000	0.014	0.007	-0.002	-0.016	-0.034	-0.525	-0.555	-0.628	-0.009	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: MG101 (12)

		6	11	12	13	14	15	16	19	20	22	25	26
		C 103	NA201	MG101	AL203	SI102	P 205	S 103	K 201	CA101	TI102	MN203	FE203
	A1	0.618	2.844	0.000	0.155	0.302	0.409	0.518	0.735	0.941	1.308	2.638	3.054
	A2	-0.000	-0.000	0.000	-0.049	-0.065	-0.084	-0.103	-0.207	-0.212	-0.199	-0.041	-0.040
AIJK	6 C 103	0.000											
	11 NA201	0.000											
	12 MG101	0.000	0.000										
	13 AL203	-0.010	-0.037	0.000									
	14 SI102	-0.011	-0.045	0.000	0.063								
	15 P 205	-0.014	-0.059	0.000	0.082	0.084							
	16 S 103	-0.019	-0.075	0.000	0.101	0.103	0.109						
	19 K 201	-0.207	-0.479	0.000	0.211	0.215	0.239	0.257					
	20 CA101	-0.216	-0.504	0.000	0.213	0.216	0.240	0.258	0.556				
	22 TI102	-0.245	-0.567	0.000	0.194	0.196	0.219	0.236	0.542	0.539			
	25 MN203	-0.014	-0.043	0.000	0.008	0.003	-0.005	-0.015	-0.319	-0.340	-0.389		
	26 FE203	-0.013	-0.041	0.000	0.003	-0.003	-0.012	-0.024	-0.360	-0.383	-0.439	-0.007	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: AL2O3 (13)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 1O3	NA2O1	MG1O1	AL2O3	SI1O2	P 2O5	S 1O3	K 2O1	CA1O1	TI1O2	MN2O3	FE2O3
		A1	0.342	2.201	2.508	0.000	0.103	0.194	0.285	0.512	0.679	0.980	2.058	2.408
		A2	-0.000	-0.000	-0.000	0.000	-0.056	-0.073	-0.089	-0.186	-0.186	-0.169	-0.033	-0.032
AIJK	6	C 1O3	0.000											
	11	NA2O1	0.000											
	12	MG1O1	0.000	0.000										
	13	AL2O3	0.000	0.000	0.000									
	14	SI1O2	-0.008	-0.037	-0.041	0.000								
	15	P 2O5	-0.010	-0.049	-0.053	0.000	0.073							
	16	S 1O3	-0.013	-0.061	-0.067	0.000	0.089	0.094						
	19	K 2O1	-0.154	-0.376	-0.404	0.000	0.198	0.219	0.235					
	20	CA1O1	-0.163	-0.398	-0.427	0.000	0.196	0.216	0.232	0.499				
	22	TI1O2	-0.190	-0.452	-0.486	0.000	0.174	0.194	0.209	0.483	0.479			
	25	MN2O3	-0.011	-0.035	-0.038	0.000	0.001	-0.006	-0.014	-0.250	-0.269	-0.312		
	26	FE2O3	-0.010	-0.033	-0.036	0.000	-0.004	-0.012	-0.021	-0.284	-0.305	-0.354	-0.006	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: SI102 (14)

		6	11	12	13	14	15	16	19	20	22	25	26
		C 103	NA201	MG101	AL203	SI102	P 205	S 103	K 201	CA101	TI102	MN203	FE203
	A1	0.151	1.756	2.022	2.350	0.000	0.055	0.135	0.389	0.527	0.781	1.655	1.960
	A2	-0.000	-0.001	-0.001	-0.001	0.000	-0.066	-0.081	-0.185	-0.181	-0.160	-0.028	-0.027
AIJK	6 C 103	0.000											
	11 NA201	0.000											
	12 MG101	0.000	0.000										
	13 AL203	0.000	0.000	0.000									
	14 SI102	0.000	0.000	0.000	0.000								
	15 P 205	-0.006	-0.040	-0.045	-0.049	0.000							
	16 S 103	-0.008	-0.051	-0.056	-0.061	0.000	0.086						
	19 K 201	-0.110	-0.297	-0.321	-0.349	0.000	0.215	0.230					
	20 CA101	-0.120	-0.317	-0.343	-0.372	0.000	0.209	0.224	0.476				
	22 TI102	-0.146	-0.367	-0.396	-0.430	0.000	0.184	0.198	0.457	0.451			
	25 MN203	-0.009	-0.030	-0.033	-0.036	0.000	-0.005	-0.012	-0.194	-0.212	-0.253		
	26 FE203	-0.008	-0.028	-0.031	-0.034	0.000	-0.011	-0.019	-0.224	-0.243	-0.288	-0.005	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: P 205 (15)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 103	NA201	MG101	AL203	SI102	P 205	S 103	K 201	CA101	TI102	MN203	FE203
		A1	0.012	1.432	1.669	1.961	2.225	0.000	0.040	0.346	0.462	0.680	1.364	1.635
		A2	-0.001	-0.001	-0.001	-0.002	-0.002	0.000	-0.077	-0.207	-0.199	-0.176	-0.025	-0.024
AIJK	6	C 103	0.000											
	11	NA201	0.000											
	12	MG101	0.000	0.000										
	13	AL203	0.000	0.000	-0.000									
	14	SI102	0.000	0.000	-0.000	0.000								
	15	P 205	0.000	0.000	0.000	0.000	0.000							
	16	S 103	-0.003	-0.042	-0.046	-0.052	-0.056	0.000						
	19	K 201	-0.065	-0.226	-0.247	-0.271	-0.292	0.000	0.234					
	20	CA101	-0.077	-0.246	-0.268	-0.294	-0.316	0.000	0.225	0.469				
	22	TI102	-0.103	-0.292	-0.318	-0.348	-0.373	0.000	0.198	0.451	0.443			
	25	MN203	-0.007	-0.026	-0.029	-0.032	-0.034	0.000	-0.010	-0.141	-0.159	-0.197		
	26	FE203	-0.007	-0.025	-0.027	-0.030	-0.032	0.000	-0.016	-0.167	-0.186	-0.228	-0.004	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: S 103 (16)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 103	NA201	MG101	AL203	SI102	P 205	S 103	K 201	CA101	TI102	MN203	FE203
		A1	-0.114	1.137	1.346	1.605	1.839	2.155	0.000	0.319	0.413	0.598	1.093	1.332
		A2	-0.001	-0.002	-0.003	-0.003	-0.003	-0.003	0.000	-0.230	-0.219	-0.193	-0.022	-0.022
AIJK	6	C 103	0.000											
	11	NA201	0.000											
	12	MG101	0.000	0.000										
	13	AL203	0.000	0.000	0.000									
	14	SI102	0.000	0.000	0.000	-0.000								
	15	P 205	0.000	0.000	0.000	0.000	0.000							
	16	S 103	0.000	0.000	0.000	0.000	0.000	0.000						
	19	K 201	-0.022	-0.156	-0.174	-0.194	-0.212	-0.234	0.000					
	20	CA101	-0.035	-0.176	-0.195	-0.217	-0.236	-0.260	0.000	0.472				
	22	TI102	-0.062	-0.220	-0.242	-0.268	-0.289	-0.317	0.000	0.457	0.447			
	25	MN203	-0.006	-0.023	-0.025	-0.028	-0.030	-0.033	0.000	-0.085	-0.104	-0.140		
	26	FE203	-0.006	-0.022	-0.024	-0.027	-0.029	-0.031	0.000	-0.108	-0.127	-0.167	-0.004	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: K 201 (19)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 103	NA201	MG101	AL203	SI102	P 205	S 103	K 201	CA101	TI102	MN203	FE203
		A1	-0.609	-0.052	0.042	0.159	0.265	0.408	0.529	0.000	-0.052	0.032	-0.041	0.064
		A2	-0.008	-0.021	-0.023	-0.025	-0.027	-0.029	-0.031	0.000	-0.197	-0.211	-0.037	-0.036
AIJK	6	C 103	0.000											
	11	NA201	0.001											
	12	MG101	0.001	0.000										
	13	AL203	0.002	0.000	0.000									
	14	SI102	0.002	0.000	0.000	0.000								
	15	P 205	0.002	0.000	0.000	0.000	0.000							
	16	S 103	0.002	0.000	0.000	0.000	0.000	0.000						
	19	K 201	0.000	0.000	0.000	0.000	0.000	0.000	0.000					
	20	CA101	0.067	0.023	0.017	0.009	0.002	-0.007	-0.015	0.000				
	22	TI102	0.066	0.016	0.009	-0.000	-0.008	-0.019	-0.027	0.000	0.226			
	25	MN203	0.002	-0.006	-0.007	-0.008	-0.009	-0.011	-0.012	0.000	0.044	0.040		
	26	FE203	0.002	-0.006	-0.007	-0.009	-0.010	-0.011	-0.012	0.000	0.035	0.029	-0.001	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: CA101 (20)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 103	NA201	MG101	AL203	SI102	P 205	S 103	K 201	CA101	TI102	MN203	FE203
		A1	-0.672	-0.202	-0.123	-0.024	0.066	0.187	0.289	2.518	0.000	-0.034	-0.186	-0.098
		A2	-0.008	-0.021	-0.023	-0.025	-0.027	-0.029	-0.031	-0.059	0.000	-0.208	-0.037	-0.035
AIJK	6	C 103	0.000											
	11	NA201	0.001											
	12	MG101	0.001	0.000										
	13	AL203	0.002	0.000	0.000									
	14	SI102	0.002	0.000	0.000	0.000								
	15	P 205	0.002	0.000	0.000	0.000	0.000							
	16	S 103	0.003	0.000	0.000	0.000	0.000	0.000						
	19	K 201	0.006	0.002	0.002	0.002	0.001	0.001	0.001					
	20	CA101	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000				
	22	TI102	0.078	0.043	0.038	0.032	0.026	0.019	0.013	-0.083	0.000			
	25	MN203	0.002	-0.005	-0.006	-0.007	-0.008	-0.009	-0.010	-0.023	0.000	0.067		
	26	FE203	0.002	-0.006	-0.007	-0.008	-0.009	-0.010	-0.011	-0.023	0.000	0.058	-0.000	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: TI1O2 (22)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 1O3	NA2O1	MG1O1	AL2O3	SI1O2	P 2O5	S 1O3	K 2O1	CA1O1	TI1O2	MN2O3	FE2O3
		A1	-0.767	-0.431	-0.373	-0.302	-0.238	-0.151	-0.076	1.523	1.513	0.000	-0.405	-0.344
		A2	-0.008	-0.022	-0.024	-0.026	-0.029	-0.031	-0.034	-0.067	-0.067	0.000	-0.042	-0.039
AIJK	6	C 1O3	0.000											
	11	NA2O1	0.001											
	12	MG1O1	0.002	0.000										
	13	AL2O3	0.002	0.000	0.000									
	14	SI1O2	0.002	0.000	0.000	0.000								
	15	P 2O5	0.003	0.000	0.000	0.000	0.000							
	16	S 1O3	0.003	0.000	0.000	0.000	0.000	0.000						
	19	K 2O1	0.008	0.003	0.003	0.002	0.002	0.002	0.001					
	20	CA1O1	0.008	0.003	0.003	0.002	0.002	0.002	0.001	0.000				
	22	TI1O2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000			
	25	MN2O3	0.005	-0.002	-0.003	-0.004	-0.004	-0.005	-0.006	-0.015	-0.015	0.000		
	26	FE2O3	0.003	-0.004	-0.004	-0.005	-0.006	-0.007	-0.008	-0.017	-0.017	0.000	0.001	

HYBRID ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: MN2O3 (25)

			6	11	12	13	14	15	16	19	20	22	25	26
			C 1O3	NA2O1	MG1O1	AL2O3	SI1O2	P 2O5	S 1O3	K 2O1	CA1O1	TI1O2	MN2O3	FE2O3
		A1	-0.706	-0.275	-0.201	-0.109	-0.025	0.088	0.185	2.265	2.255	2.523	0.000	0.114
		A2	-0.008	-0.026	-0.029	-0.033	-0.036	-0.040	-0.044	-0.103	-0.103	-0.108	0.000	-0.001
AIJK	6	C 1O3	0.000											
	11	NA2O1	0.002											
	12	MG1O1	0.003	0.000										
	13	AL2O3	0.004	0.000	0.000									
	14	SI1O2	0.005	0.000	0.000	0.000								
	15	P 2O5	0.006	0.001	0.000	0.000	0.000							
	16	S 1O3	0.006	0.001	0.001	0.000	0.000	0.000						
	19	K 2O1	0.018	0.008	0.007	0.006	0.005	0.004	0.004					
	20	CA1O1	0.018	0.008	0.007	0.006	0.005	0.004	0.004	0.000				
	22	TI1O2	0.019	0.008	0.007	0.006	0.006	0.005	0.004	0.000	0.000			
	25	MN2O3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
	26	FE2O3	0.008	0.026	0.029	0.033	0.036	0.041	0.044	0.096	0.096	0.100	0.000	

HYBRID ALPHA COEFFICIENTS FOR JSE IN COLA EQUATION

(OXIDE SYSTEM)

TARGET: CR 45.0 KV
GEOMETRY: 55,35 DEGREES

ANALYTE: FE2O3 (26)

		6	11	12	13	14	15	16	19	20	22	25	26
		C 1O3	NA2O1	MG1O1	AL2O3	SI1O2	P 2O5	S 1O3	K 2O1	CA1O1	TI1O2	MN2O3	FE2O3
	A1	-0.804	-0.517	-0.468	-0.406	-0.350	-0.274	-0.210	1.160	1.154	1.330	-0.101	0.000
	A2	-0.012	-0.040	-0.045	-0.051	-0.057	-0.064	-0.070	-0.179	-0.178	-0.189	-0.000	0.000
AIJK	6 C 1O3	0.000											
	11 NA2O1	0.004											
	12 MG1O1	0.006	0.000										
	13 AL2O3	0.007	0.000	0.000									
	14 SI1O2	0.008	0.001	0.000	0.000								
	15 P 2O5	0.010	0.001	0.001	0.000	0.000							
	16 S 1O3	0.012	0.002	0.001	0.001	0.000	0.000						
	19 K 2O1	0.036	0.017	0.015	0.013	0.011	0.009	0.008					
	20 CA1O1	0.036	0.017	0.015	0.013	0.011	0.009	0.008	-0.000				
	22 TI1O2	0.038	0.018	0.016	0.014	0.012	0.010	0.009	0.000	0.000			
	25 MN2O3	0.011	0.039	0.044	0.051	0.056	0.063	0.069	0.160	0.159	0.167		
	26 FE2O3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	

3.3B Calculated Compositions of Cement Samples Using Different Calibration Curves

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$RUN CALCOMP


DATE:  03-OCT-84      TIME:  13:35:08

WHAT TYPE OF UNKNOWNS DO YOU WISH TO ANALYZE :
  1-ELEMENT SYSTEM    2-OXIDE SYSTEM    3-FUSED DISK SYSTEM  ?  2
DO YOU WANT TO INPUT KNOWN CONCENTRATIONS OF UNANALYZED ELEMENTS (Y/N)?  Y
INPUT N6(NUMBER OF ALL CONSTITUENTS), N(NUMBER OF ANALYTES) AND
  M(NUMBER OF SPECIMENS TO BE ANALYZED) :          12,8,2
INPUT NAMES OF CONSTITUENTS(XXXXXXXX)(MAX.=8/LINE) :

LOI     NA2O    MGO     AL2O3   SIO2    P2O5    SO3     K2O
CAO     TIO2    MN2O3   FE2O3
INPUT NAMES OF ANALYTES(XXXXXXXX)(MAX.=8/LINE) :

AL2O3   SIO2    SO3     K2O     CAO     TIO2    MN2O3   FE2O3
DO YOU WANT TO INPUT ALPHA COEFFICIENTS BY: 1-DATAFILE  2-KEYBOARD  ?  1
INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX) :  OXCEMT.C45
WHAT TYPE OF STANDARDS ARE AVAILABLE: 1-PURE STANDARDS    2-MULTIELEMENT STANDARDS  ?  2
INPUT M1(NUMBER OF STANDARDS) :  7
INPUT I.D. OF STANDARDS (<=8 CHARACTERS) :

 I= 1    633
 I= 2    634
 I= 3    635
 I= 4    636
 I= 5    637
 I= 6    638
 I= 7    639
INPUT CONCENTRATIONS(WEIGHT FRACTION) OF STANDARDS :

 I= 1    633       .0075,.0064,.0104,.0378,.2188,.0024,.0220,.0017,.6450,.0024,.0004,.0420
 I= 2    634       .0162,.0015,.0330,.0521,.2073,.0010,.0221,.0042,.6258,.0029,.0028,.0284
 I= 3    635       .0324,.0007,.0123,.0629,.1841,.0017,.0707,.0045,.5983,.0032,.0009,.0261
 I= 4    636       .0116,.0011,.0395,.0302,.2322,.0008,.0231,.0059,.6354,.0018,.0012,.0161
 I= 5    637       .0169,.0015,.0067,.0328,.2307,.0024,.0238,.0025,.6504,.0021,.0006,.0180
 I= 6    638       .0095,.0013,.0383,.0445,.2148,.0006,.0234,.0059,.6209,.0025,.0005,.0355
 I= 7    639       .0100,.0065,.0126,.0428,.2161,.0008,.0248,.0006,.6576,.0032,.0008,.0240
INPUT NET INTENSITIES FOLLOWED BY A PERIOD FOR THE ANALYTE ELEMENTS IN STANDARDS AND
  ENTER 0.0 FOR EACH UNANALYZED ELEMENT:

 I= 1    633       3*0.0,277\7\22.,20360.,0.0,6017.,11983.,149102.,7902.,46.,28869.
 I= 2    634       3*0.0,3761.,19134.,0.0,5913.,31595.,145546.,9590.,329.,20078.
 I= 3    635       3*0.0,4886.,17241.,0.0,19390.,32989.,138586.,10675.,106.,19107.
 I= 4    636       3*0.0,2295.,21785.,0.0,6310.,41964.,146070.,5504.,128.,11504.
 I= 5    637       3*0.0,2450.,22113.,0.0,6433.,18455.,153049.,6619.,65.,12363.
 I= 6    638       3*0.0,3195.,19743.,0.0,6244.,43312.,143465.,8363.,56.,25258.
 I= 7    639       3*0.0,3140.,20348.,0.0,6832.,3794.,153133.,10041.,91.,16592.
INPUT I.D. OF SPECIMENS TO BE ANALYZED :

 I= 1    BLACK
 I= 2    WHITE
INPUT NET INTENSITIES FOR ANALYTES IN SPECIMENS AND
  ENTER CONCENTRATIONS(WEIGHT FRACTION) FOR UNANALYZED ELEMENTS:

 I= 1    BLACK     .0139,.0028,.0269,3669.,18475.,.0029,9174.,65774.,144509.,7806.,97.,20489.
 I= 2    WHITE     .0201,.0004,.0262,3134.,20372.,.0009,9955.,82080.,134125.,6881.,318.,33818.
DO YOU WANT TO CORRECT INTENSITIES FOR DEAD TIME (Y/N) ?  N
DO YOU WANT TO PRINT OUT CALCULATED RELATIVE INTENSITIES OF STANDARDS &
  CALCULATED PURE INTENSITIES FROM STANDARDS (Y/N) ?  Y

CALCULATED RELATIVE INTENSITIES OF STANDARDS :
```

	AL2O3	SIO2	SO3	K2O	CAO	TIO2	MN2O3	FE2O3
STD.NO.=633	0.02514	0.15176	0.01350	0.00188	0.63925	0.00131	0.00017	0.02774
STD.NO.=634	0.03444	0.14023	0.01353	0.00464	0.62150	0.00161	0.00120	0.01920
STD.NO.=635	0.04305	0.12657	0.04470	0.00488	0.59127	0.00182	0.00040	0.01811
STD.NO.=636	0.02011	0.16297	0.01412	0.00649	0.62431	0.00099	0.00051	0.01082
STD.NO.=637	0.02267	0.16683	0.01484	0.00278	0.65365	0.00113	0.00025	0.01184
STD.NO.=638	0.02904	0.14514	0.01420	0.00646	0.61135	0.00139	0.00021	0.02399
STD.NO.=639	0.02896	0.15117	0.01539	0.00067	0.65342	0.00173	0.00033	0.01580

CALCULATED PURE INTENSITIES FROM STANDARDS :

	AL2O3	SIO2	SO3	K2O	CAO	TIO2	MN2O3	FE2O3
STD.NO.=633	108275.	134157.	445577.	6390643.	233244.	6033537.	273908.	1040619.
STD.NO.=634	109205.	136444.	437075.	6812073.	234183.	5945329.	274191.	1045840.
STD.NO.=635	113506.	136219.	433768.	6761152.	234385.	5849718.	267996.	1055188.
STD.NO.=636	114148.	133672.	446806.	6464833.	233970.	5569186.	251343.	1062949.
STD.NO.=637	108058.	132545.	433604.	6639349.	234146.	5862505.	260803.	1044160.
STD.NO.=638	110035.	136030.	439660.	6699596.	234668.	6004703.	261088.	1052648.
STD.NO.=639	108438.	134607.	443912.	5700546.	234358.	5811805.	273284.	1050044.
AVERAGE VALUES	110238.	134811.	440057.	6495457.	234136.	5868112.	266088.	1050207.

WHAT TYPE OF LSF CURVES DO YOU WANT TO USE FOR CALIBRATION :
(1) Y=A0+A1*X (2) Y=A0+A1*X+A2*X*X
(3) Y=A1*X (4) Y=A1*X+A2*X*X ? 4
DO YOU WANT TO PRINT OUT LSF COEFFICIENTS (Y/N) : Y

TABULATION OF CALCULATED LSF COEFFICIENTS
(X=MEAS.INT. ; Y=CALC.REL.INT.)

AL2O3	A0= 0.00000E+00	A1= 0.95139E-05	A2=-0.13075E-09
SIO2	A0= 0.00000E+00	A1= 0.64906E-05	A2= 0.46134E-10
SO3	A0= 0.00000E+00	A1= 0.22487E-05	A2= 0.29227E-11
K2O	A0= 0.00000E+00	A1= 0.14864E-06	A2= 0.49290E-13
CAO	A0= 0.00000E+00	A1= 0.42058E-05	A2= 0.44370E-12
TIO2	A0= 0.00000E+00	A1= 0.17240E-06	A2=-0.27409E-12
MN2O3	A0= 0.00000E+00	A1= 0.38786E-05	A2=-0.68945E-09
FE2O3	A0= 0.00000E+00	A1= 0.94055E-06	A2= 0.59843E-12

-----RESULTS OF LAST ITERATION-----

SMP.NO.=BLACK	R=AL2O3	0.03315	SIO2	0.13566	SO3	0.02088	K2O	0.00999	CAO	0.61704	TIO2	0.00133
	MN2O3	0.00037	FE2O3	0.01952								
L= 3	C=LOI	1.390%	NA2O	0.280%	MGO	2.690%	AL2O3	4.998%	SIO2	19.922%	P2O5	0.290%
	SO3	3.375%	K2O	0.908%	CAO	63.229%	TIO2	0.242%	MN2O3	0.087%	FE2O3	2.916%
	TOTAL= 100.34%											
SMP.NO.=WHITE	R=AL2O3	0.02853	SIO2	0.15137	SO3	0.02267	K2O	0.01253	CAO	0.57209	TIO2	0.00117
	MN2O3	0.00116	FE2O3	0.03249								
L= 3	C=LOI	2.010%	NA2O	0.040%	MGO	2.620%	AL2O3	4.356%	SIO2	22.296%	P2O5	0.090%
	SO3	3.760%	K2O	1.157%	CAO	58.737%	TIO2	0.204%	MN2O3	0.264%	FE2O3	4.691%
	TOTAL= 100.23%											

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	LOI	NA2O	MGO	AL2O3	SIO2	P2O5	SO3	K2O	CAO	TIO2	MN2O3	FE2O3
BLACK	100.34	1.390	0.280	2.690	4.998	19.922	0.290	3.375	0.908	63.229	0.242	0.087	2.916

```
WHITE     100.23  2.010   0.040   2.620   4.356  22.296   0.090   3.760   1.157  58.737   0.204   0.264   4.691


DO YOU WISH TO COMPARE THESE RESULTS WITH OTHER PREVIOUSLY KNOWN VALUES FOR THESE SPECIMENS (Y/N) ?  Y
ENTER KNOWN CONCENTRATIONS OF SPECIMENS :

SMP.NO.=BLACK     .0139,.0028,.0269,.0502,.1982,.0029,.0337,.0091,.6315,.0023,.0008,.0291
SMP.NO.=WHITE     .0201,.0004,.0262,.0418,.2225,.0009,.0365,.0117,.5869,.0024,.0026,.0468

                                    TABULATION OF RESULTS (%)

SMP.NO.   TOTAL   LOI     NA2O    MGO     AL2O3   SIO2    P2O5    SO3     K2O     CAO     TIO2    MN2O3   FE2O3

BLACK      100.14  1.39    0.28    2.69    5.02   19.82    0.29    3.37    0.91   63.15    0.23    0.08    2.91
           100.34  1.39    0.28    2.69    5.00   19.92    0.29    3.38    0.91   63.23    0.24    0.09    2.92
        ABS.ERR.   0.00    0.00    0.00   -0.02    0.10    0.00    0.01    0.00    0.08    0.01    0.01    0.01
        REL.ERR.   0.00    0.00    0.00   -0.40    0.50    0.00    0.30    0.00    0.13    4.35   12.50    0.34

WHITE      99.87   2.01    0.04    2.62    4.18   22.25    0.09    3.65    1.17   58.68    0.24    0.26    4.68
           100.23  2.01    0.04    2.62    4.36   22.30    0.09    3.76    1.16   58.74    0.20    0.26    4.69
        ABS.ERR.   0.00    0.00    0.00    0.18    0.05    0.00    0.11   -0.01    0.06   -0.04    0.00    0.01
        REL.ERR.   0.00    0.00    0.00    4.31    0.22    0.00    3.01   -0.85    0.10  -16.67    0.00    0.21


    AVG.ABS.ERR.   0.00    0.00    0.00    0.10    0.07    0.00    0.06    0.00    0.07    0.02    0.01    0.01
    AVG.REL.ERR.   0.00    0.00    0.00    2.35    0.36    0.00    1.66    0.43    0.11   10.51    6.25    0.28


DO YOU WANT TO TRY ANOTHER TYPE OF CALIBRATION CURVE (Y/N) ?  Y

WHAT TYPE OF LSF CURVES DO YOU WANT TO USE FOR CALIBRATION :
  (1) Y=A0+A1*X       (2) Y=A0+A1*X+A2*X*X
  (3) Y=A1*X          (4) Y=A1*X+A2*X*X       ?  3
DO YOU WANT TO PRINT OUT LSF COEFFICIENTS (Y/N) :  Y

              TABULATION OF CALCULATED LSF COEFFICIENTS
                 (X=MEAS.INT.  ;  Y=CALC.REL.INT.)

AL2O3     A0= 0.00000E+00  A1= 0.90363E-05  A2= 0.00000E+00
SIO2      A0= 0.00000E+00  A1= 0.74285E-05  A2= 0.00000E+00
SO3       A0= 0.00000E+00  A1= 0.22905E-05  A2= 0.00000E+00
K2O       A0= 0.00000E+00  A1= 0.15046E-06  A2= 0.00000E+00
CAO       A0= 0.00000E+00  A1= 0.42712E-05  A2= 0.00000E+00
TIO2      A0= 0.00000E+00  A1= 0.16992E-06  A2= 0.00000E+00
MN2O3     A0= 0.00000E+00  A1= 0.36982E-05  A2= 0.00000E+00
FE2O3     A0= 0.00000E+00  A1= 0.95406E-06  A2= 0.00000E+00

-----RESULTS OF LAST ITERATION-----

SMP.NO.=BLACK     R=AL2O3   0.03315 SIO2    0.13724 SO3     0.02101 K2O     0.00990 CAO     0.61722 TIO2    0.00133
                  MN2O3     0.00036 FE2O3   0.01955
            L= 3  C=LOI      1.390% NA2O     0.280% MGO      2.690% AL2O3    4.999% SIO2    20.155% P2O5     0.290%
                  SO3        3.405% K2O     0.900% CAO     63.247% TIO2     0.241% MN2O3    0.085% FE2O3    2.917%

                  TOTAL= 100.60%

SMP.NO.=WHITE     R=AL2O3   0.02832 SIO2    0.15133 SO3     0.02280 K2O     0.01235 CAO     0.57287 TIO2    0.00117
                  MN2O3     0.00118 FE2O3   0.03226
            L= 3  C=LOI      2.010% NA2O     0.040% MGO      2.620% AL2O3    4.322% SIO2    22.274% P2O5     0.090%
                  SO3        3.778% K2O     1.140% CAO     58.799% TIO2     0.204% MN2O3    0.267% FE2O3    4.660%
```

TOTAL= 100.20%

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	LOI	NA2O	MGO	AL2O3	SIO2	P2O5	SO3	K2O	CAO	TIO2	MN2O3	FE2O3
BLACK	100.60	1.390	0.280	2.690	4.999	20.155	0.290	3.405	0.900	63.247	0.241	0.085	2.917
WHITE	100.20	2.010	0.040	2.620	4.322	22.274	0.090	3.778	1.140	58.799	0.204	0.267	4.660

DO YOU WISH TO COMPARE THESE RESULTS WITH OTHER PREVIOUSLY KNOWN VALUES FOR THESE SPECIMENS (Y/N) ? Y

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	LOI	NA2O	MGO	AL2O3	SIO2	P2O5	SO3	K2O	CAO	TIO2	MN2O3	FE2O3
BLACK	100.14	1.39	0.28	2.69	5.02	19.82	0.29	3.37	0.91	63.15	0.23	0.08	2.91
	100.60	1.39	0.28	2.69	5.00	20.15	0.29	3.41	0.90	63.25	0.24	0.08	2.92
	ABS.ERR.	0.00	0.00	0.00	-0.02	0.33	0.00	0.04	-0.01	0.10	0.01	0.00	0.01
	REL.ERR.	0.00	0.00	0.00	-0.40	1.65	0.00	1.19	-1.10	0.16	4.35	0.00	0.34
WHITE	99.87	2.01	0.04	2.62	4.18	22.25	0.09	3.65	1.17	58.68	0.24	0.26	4.68
	100.20	2.01	0.04	2.62	4.32	22.27	0.09	3.78	1.14	58.80	0.20	0.27	4.66
	ABS.ERR.	0.00	0.00	0.00	0.14	0.02	0.00	0.13	-0.03	0.12	-0.04	0.01	-0.02
	REL.ERR.	0.00	0.00	0.00	3.35	0.09	0.00	3.56	-2.56	0.20	-16.67	3.85	-0.43
	AVG.ABS.ERR.	0.00	0.00	0.00	0.08	0.18	0.00	0.09	0.02	0.11	0.02	0.01	0.01
	AVG.REL.ERR.	0.00	0.00	0.00	1.87	0.88	0.00	2.37	1.83	0.18	10.51	1.92	0.39

DO YOU WANT TO TRY ANOTHER TYPE OF CALIBRATION CURVE (Y/N) ? N

TTO — STOP

3.4A Calculation of Coefficients for Fused Rock Samples

```
$RUN CALCO


DATE:  03-OCT-84      TIME:  08:45:48

WHICH SYSTEM DO YOU WISH TO ANALYZE:
  1-ELEMENT SYSTEM  2-OXIDE SYSTEM  3-FUSED DISK SYSTEM  ?  3
INPUT NUMBER OF ANALYTES:  12
INPUT NAMES OF ANALYTES (XXNONS):

NA201 MG101 AL203 SI102 P 205 S 103 K 201 CA101 TI102 CR203 MN101 FE203
WHAT MASS ABS. COEF. ALGORITHM DO YOU WANT TO USE :
  1-LEROUX ALGORITHM  2-HEINRICH ALGORITHM ?  2
DO YOU WANT TO CREATE A DATAFILE FOR SAVING CALCULATED ALPHA COEFFICIENTS (Y/N)?  Y
INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX) :  FDROCK.C60
INPUT MEAN CONCENTRATIONS (WEIGHT FRACTION) OF ANALYTES IN THE SPECIMENS TO BE ANALYZED:
  I= 1    NA201    .05
  I= 2    MG101    .25
  I= 3    AL203    .30
  I= 4    SI102    .50
  I= 5    P 205    .005
  I= 6    S 103    .015
  I= 7    K 201    .075
  I= 8    CA101    .175
  I= 9    TI102    .015
  I=10    CR203    .010
  I=11    MN101    .005
  I=12    FE203    .40
FOR SAMPLE GEOMETRY, INPUT INCIDENCE & EMERGENCE ANGLES (DEGREE-XX):  55,35
INPUT THE CHARACTERISTIC LINE NUMBER YOU WISH TO MEASURE (1-KA, 2-KB, 3-LA1, 4-LB1, 5-LB2):
I= 1    NA    1
I= 2    MG    1
I= 3    AL    1
I= 4    SI    1
I= 5    P     1
I= 6    S     1
I= 7    K     1
I= 8    CA    1
I= 9    TI    1
I=10    CR    1
I=11    MN    1
I=12    FE    1
DO YOU WANT TO PRINT OUT CALCULATED ALPHA COEFFICIENTS(Y/N):  Y
WHICH X-RAY TUBE SPECTRAL DISTRIBUTION DO YOU PREFER:
  1-CALCULATED SPECTRUM FROM NBS ALGORITHM  ;  2-MEASURED SPECTRUM ?  1
DO YOU WANT TO PRINT OUT THE SPECTRAL DISTRIBUTION(Y/N) ?  Y
INPUT NAME OF X-RAY TUBE TARGET (XX) :  CR
INPUT VOLTAGE(KV), TAKE-OFF ANGLE OF X-RAY FROM TUBE TARGET(DEGREE), AND
   WINDOW THICKNESS(MM) OF X-RAY TUBE :  60.0,26.0,.45
INPUT THE ENDING WAVELENGTH OF X-RAY TUBE SPECTRUM(ANGSTROM) :  2.99
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CALCULATED X-RAY TUBE SPECTRAL DISTRIBUTION
USING NBS ALGORITHM

X-RAY TUBE TARGET: CR KV: 60.0
TAKE-OFF ANGLE(DEGREE): 26.0 BE WINDOW THICKNESS(MM): 0.450

LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A	LAMDA(A)	I*.02A
0.2066	0.0000E+00	0.2266	0.1229E-03	0.2466	0.2072E-03	0.2666	0.2656E-03	0.2866	0.3059E-03
0.3066	0.3334E-03	0.3266	0.3518E-03	0.3466	0.3634E-03	0.3666	0.3702E-03	0.3866	0.3733E-03
0.4066	0.3736E-03	0.4266	0.3718E-03	0.4466	0.3685E-03	0.4666	0.3640E-03	0.4866	0.3596E-03
0.5066	0.3525E-03	0.5266	0.3459E-03	0.5466	0.3390E-03	0.5666	0.3318E-03	0.5866	0.3244E-03
0.6066	0.3169E-03	0.6266	0.3093E-03	0.6466	0.3018E-03	0.6666	0.2942E-03	0.6866	0.2867E-03
0.7066	0.2792E-03	0.7266	0.2718E-03	0.7466	0.2645E-03	0.7666	0.2573E-03	0.7866	0.2502E-03
0.8066	0.2432E-03	0.8266	0.2363E-03	0.8466	0.2296E-03	0.8666	0.2230E-03	0.8866	0.2165E-03
0.9066	0.2101E-03	0.9266	0.2039E-03	0.9466	0.1978E-03	0.9666	0.1919E-03	0.9866	0.1860E-03
1.0066	0.1804E-03	1.0266	0.1748E-03	1.0466	0.1694E-03	1.0666	0.1641E-03	1.0866	0.1590E-03
1.1066	0.1540E-03	1.1266	0.1491E-03	1.1466	0.1444E-03	1.1666	0.1397E-03	1.1866	0.1352E-03
1.2066	0.1309E-03	1.2266	0.1266E-03	1.2466	0.1225E-03	1.2666	0.1185E-03	1.2866	0.1146E-03
1.3066	0.1109E-03	1.3266	0.1072E-03	1.3466	0.1037E-03	1.3666	0.1002E-03	1.3866	0.9690E-04
1.4066	0.9367E-04	1.4266	0.9055E-04	1.4466	0.8753E-04	1.4666	0.8461E-04	1.4866	0.8178E-04
1.5066	0.7904E-04	1.5266	0.7639E-04	1.5466	0.7384E-04	1.5666	0.7136E-04	1.5866	0.6897E-04
1.6066	0.6666E-04	1.6266	0.6443E-04	1.6466	0.6228E-04	1.6666	0.6020E-04	1.6866	0.5819E-04
1.7066	0.5625E-04	1.7266	0.5437E-04	1.7466	0.5257E-04	1.7666	0.5082E-04	1.7866	0.4913E-04
1.8066	0.4751E-04	1.8266	0.4594E-04	1.8466	0.4442E-04	1.8666	0.4296E-04	1.8866	0.4155E-04
1.9066	0.4019E-04	1.9266	0.3888E-04	1.9466	0.3761E-04	1.9666	0.3639E-04	1.9866	0.3521E-04
2.0066	0.3407E-04	2.0266	0.3297E-04	2.0466	0.3191E-04	2.0666	0.3089E-04	2.0866	0.8238E-04
2.1066	0.8063E-04	2.1266	0.7891E-04	2.1466	0.7722E-04	2.1666	0.7556E-04	2.1866	0.7393E-04
2.2066	0.7232E-04	2.2266	0.7073E-04	2.2466	0.6918E-04	2.2666	0.6765E-04	2.2866	0.6614E-04
2.3066	0.6466E-04	2.3266	0.6321E-04	2.3466	0.6178E-04	2.3666	0.6037E-04	2.3866	0.5899E-04
2.4066	0.5763E-04	2.4266	0.5630E-04	2.4466	0.5499E-04	2.4666	0.5370E-04	2.4866	0.5244E-04
2.5066	0.5120E-04	2.5266	0.4998E-04	2.5466	0.4878E-04	2.5666	0.4761E-04	2.5866	0.4646E-04
2.6066	0.4533E-04	2.6266	0.4422E-04	2.6466	0.4313E-04	2.6666	0.4207E-04	2.6866	0.4102E-04
2.7066	0.3999E-04	2.7266	0.3899E-04	2.7466	0.3800E-04	2.7666	0.3704E-04	2.7866	0.3609E-04
2.8066	0.3516E-04	2.8266	0.3425E-04	2.8466	0.3336E-04	2.8666	0.3249E-04	2.8866	0.3164E-04
2.9066	0.3080E-04	2.9266	0.2999E-04	2.9466	0.2919E-04	2.9666	0.2840E-04	2.9866	0.2764E-04

KA	KB	LA1	LB1	LB2	LB3	LB4	LG1	LG2	LG3	LL
2.2910	2.0850	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.3167E-01	0.5064E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

What Flux Conditions Do You Wish:

1 - Sample + Li2B407
2 - Sample + Li2B407 + LiF
3 - Sample + Li2B407 + LiBO2? 2
Grams of Sample: 1.000
Grams of Li2B407: 5.000
Grams of LiF: 0.3

MODIFIED ALPHA COEFFICIENTS FOR USE IN COLA EQUATION

(FUSED DISK SYSTEM)

TARGET: CR 60.0 KV
GEOMETRY: 55,35 DEGREES

MATRIX CONSTITUENTS

			11	12	13	14	15	16	19	20	22	24	25	26
		LOI	NA2O1	MG1O1	AL2O3	SI1O2	P 2O5	S 1O3	K 2O1	CA1O1	TI1O2	CR2O3	MN1O1	FE2O3
MEAN CONC.		50.00	5.00	25.00	30.00	50.00	0.50	1.50	7.50	17.50	1.50	1.00	0.50	40.00
ANALYTE														
11	NA2O1	-0.089	0.000	0.027	0.046	0.062	0.072	0.082	0.056	0.078	0.119	0.307	0.381	0.408
12	MG1O1	-0.122	0.346	0.000	0.011	0.027	0.036	0.046	0.026	0.047	0.086	0.266	0.338	0.364
13	AL2O3	-0.143	0.315	0.359	0.000	0.005	0.015	0.024	0.011	0.032	0.069	0.240	0.312	0.338
14	SI1O2	-0.163	0.286	0.330	0.383	0.000	-0.003	0.007	0.004	0.023	0.058	0.216	0.288	0.313
15	P 2O5	-0.181	0.259	0.302	0.355	0.403	0.000	-0.013	-0.007	0.012	0.051	0.193	0.265	0.289
16	S 1O3	-0.202	0.229	0.271	0.324	0.371	0.435	0.000	-0.009	0.009	0.046	0.167	0.238	0.262
19	K 2O1	-0.372	-0.031	0.004	0.046	0.084	0.136	0.181	0.000	-0.112	-0.087	-0.072	-0.015	0.004
20	CA1O1	-0.415	-0.096	-0.064	-0.024	0.012	0.061	0.102	1.009	0.000	-0.103	-0.133	-0.079	-0.061
22	TI1O2	-0.503	-0.233	-0.205	-0.171	-0.140	-0.098	-0.062	0.719	0.714	0.000	-0.261	-0.215	-0.201
24	CR2O3	-0.396	-0.066	-0.032	0.010	0.049	0.101	0.145	1.108	1.103	1.227	0.000	0.082	-0.298
25	MN1O1	-0.454	-0.158	-0.127	-0.089	-0.054	-0.007	0.033	0.907	0.903	1.016	-0.079	0.000	0.016
26	FE2O3	-0.548	-0.302	-0.277	-0.245	-0.216	-0.177	-0.143	0.579	0.576	0.670	1.159	-0.013	0.000

* FUSED DISK : 1 G SAMPLE + 5 G LI2B4O7 + .3 G LIF

3.4B Calculated Compositions of Fused Rock Samples

```
$RUN CALCOMP


DATE:  03-OCT-84      TIME:  10:07:34

WHAT TYPE OF UNKNOWNS DO YOU WISH TO ANALYZE :
  1-ELEMENT SYSTEM    2-OXIDE SYSTEM    3-FUSED DISK SYSTEM  ?  3
DO YOU WANT TO INPUT KNOWN CONCENTRATIONS OF UNANALYZED ELEMENTS (Y/N)?  Y
INPUT N6(NUMBER OF ALL CONSTITUENTS), N(NUMBER OF ANALYTES) AND
  M(NUMBER OF SPECIMENS TO BE ANALYZED) :          13,8,5
INPUT NAMES OF CONSTITUENTS(XXXXXXXX)(MAX.=8/LINE) :

LOI     NA2O    MGO     AL2O3   SIO2    P2O5    SO3     K2O
CAO     TIO2    CR2O3   MNO     FE2O3
INPUT NAMES OF ANALYTES(XXXXXXXX)(MAX.=8/LINE) :

NA2O    MGO     AL2O3   SIO2    K2O     CAO     TIO2    FE2O3
DO YOU WANT TO INPUT ALPHA COEFFICIENTS BY: 1-DATAFILE  2-KEYBOARD  ?  1
INPUT DATAFILE NAME OF ALPHA COEFFICIENTS(XXXXXX.XXX) :  FDROCK.C60
WHAT TYPE OF STANDARDS ARE AVAILABLE: 1-PURE STANDARDS    2-MULTIELEMENT STANDARDS  ?  2
INPUT M1(NUMBER OF STANDARDS) :  10
INPUT I.D. OF STANDARDS (<=8 CHARACTERS) :

 I= 1    SIO2
 I= 2    BCS-309
 I= 3    BCS-367
 I= 4    BR
 I= 5    NBS-77
 I= 6    NIM-D
 I= 7    NIM-P
 I= 8    NIM-S
 I= 9    NS-1
 I=10    SCH-1
INPUT CONCENTRATIONS(WEIGHT FRACTION) OF STANDARDS :

 I= 1    SIO2      3*0.0,.0005,.9972,.0001,.0010,.0002,.0003,.0001,0.0,.0001,.0005
 I= 2    BCS-309   .0008,.0034,.0017,.6110,.3410,2*0.0,.0046,.0022,.0192,0.0,.0003,.0151
 I= 3    BCS-367   0.0,.0044,.0710,.2000,.3440,.0014,.0094,.0117,.3240,.0075,0.0,.0116,.0111
 I= 4    BR        .0317,.0307,.1335,.1025,.3839,.0105,.0004,.0141,.1387,.0261,.0006,.0020,.1290
 I= 5    NBS-77    .0021,.0006,.0050,.5939,.3238,.0045,0.0,.0211,.0026,.0293,2*0.0,.0090
 I= 6    NIM-D     .0070,.0004,.4351,.0030,.3896,0.0,.0002,.0001,.0028,.0002,.0042,.0022,.1700
 I= 7    NIM-P     .0034,.0037,.2533,.0418,.5110,.0002,.0002,.0009,.0266,.0020,.0350,.0022,.1264
 I= 8    NIM-S     .0031,.0043,.0046,.1734,.6363,.0012,.0001,.1535,.0068,.0004,0.0,.0001,.0140
 I= 9    NS-1      .0081,.0989,.0065,.2130,.5337,.0028,.0001,.0651,.0173,.0106,0.0,.0019,.0420
 I=10    SCH-1     .0295,.0003,.0003,.0096,.0811,.0012,.0001,.0003,.0004,.0005,0.0,.0100,.8706
INPUT NET INTENSITIES FOLLOWED BY A PERIOD FOR THE ANALYTE ELEMENTS IN STANDARDS AND
  ENTER 0.0 FOR EACH UNANALYZED ELEMENT:

 I= 1    SIO2      0.0,7.,0.0,15.,14373.,2*0.0,166.,42.,194.,2*0.0,25.
 I= 2    BCS-309   0.0,4.,7.,6369.,4083.,2*0.0,2626.,210.,24736.,2*0.0,920.
 I= 3    BCS-367   0.0,12.,297.,2022.,4503.,2*0.0,7404.,28386.,7515.,2*0.0,491.
 I= 4    BR        0.0,64.,574.,955.,4988.,2*0.0,8719.,12693.,30193.,2*0.0,6604.
 I= 5    NBS-77    0.0,5.,17.,6183.,3945.,2*0.0,12571.,159.,37519.,2*0.0,505.
 I= 6    NIM-D     0.0,2.,1888.,21.,4776.,2*0.0,44.,288.,290.,2*0.0,10281.
 I= 7    NIM-P     0.0,9.,1112.,384.,6548.,2*0.0,537.,2480.,2422.,2*0.0,7080.
 I= 8    NIM-S     0.0,6.,21.,1776.,8658.,2*0.0,86602.,537.,506.,2*0.0,739.
 I= 9    NS-1      0.0,219.,27.,2178.,6966.,2*0.0,38381.,1417.,12295.,2*0.0,2305.
 I=10    SCH-1     0.0,2.,4.,84.,968.,2*0.0,235.,71.,738.,2*0.0,41813.
INPUT I.D. OF SPECIMENS TO BE ANALYZED :

 I= 1    BX-N
 I= 2    DT-N
 I= 3    GH
```

```
 I= 4    NBS-76
 I= 5    NBS-99A
INPUT NET INTENSITIES FOR ANALYTES IN SPECIMENS AND
  ENTER CONCENTRATIONS(WEIGHT FRACTION) FOR UNANALYZED ELEMENTS:

 I= 1    BX-N      .1217,1.,2.,5447.,889.,.0013,0.0,318.,168.,32253.,0.0,.0005,14054.
 I= 2    DT-N      .0160,0.0,2.,6126.,4456.,.0009,0.0,683.,38.,17671.,.0004,.0001,365.
 I= 3    GH        .0060,86.,2.,1326.,10501.,.0001,0.0,28146.,644.,974.,0.0,.0005,792.
 I= 4    NBS-76    .0022,7.,26.,3933.,7055.,.0007,0.0,9237.,208.,27736.,2*0.0,1308.
 I= 5    NBS-99A   .0026,148.,2.,2150.,8754.,.0002,0.0,31419.,1858.,128.,2*0.0,45.
DO YOU WANT TO CORRECT INTENSITIES FOR DEAD TIME (Y/N) ?  N
DO YOU WANT TO PRINT OUT CALCULATED RELATIVE INTENSITIES OF STANDARDS &
  CALCULATED PURE INTENSITIES FROM STANDARDS (Y/N) ?  Y

CALCULATED RELATIVE INTENSITIES OF STANDARDS :
                 NA2O      MGO       AL2O3     SIO2      K2O       CAO       TIO2      FE2O3
STD.NO.=SIO2     0.00000   0.00000   0.00050   0.99680   0.00018   0.00030   0.00012   0.00064
STD.NO.=BCS-309  0.00321   0.00166   0.60505   0.27469   0.00436   0.00222   0.02264   0.01908
STD.NO.=BCS-367  0.00411   0.06843   0.19101   0.30824   0.01166   0.32245   0.00660   0.01055
STD.NO.=BR       0.02795   0.12413   0.09270   0.33894   0.01397   0.14131   0.02719   0.13832
STD.NO.=NBS-77   0.00057   0.00489   0.58880   0.26249   0.02006   0.00258   0.03384   0.01105
STD.NO.=NIM-D    0.00036   0.40525   0.00247   0.32512   0.00010   0.00291   0.00024   0.21320
STD.NO.=NIM-P    0.00335   0.23617   0.03645   0.44494   0.00087   0.02727   0.00235   0.14630
STD.NO.=NIM-S    0.00405   0.00447   0.17129   0.59258   0.14483   0.00508   0.00040   0.01541
STD.NO.=NS-1     0.09271   0.00608   0.20253   0.47414   0.06221   0.01648   0.01164   0.04938
STD.NO.=SCH-1    0.00022   0.00023   0.00742   0.06364   0.00030   0.00043   0.00063   0.90296

CALCULATED PURE INTENSITIES FROM STANDARDS :
                 NA2O      MGO       AL2O3     SIO2      K2O       CAO       TIO2      FE2O3
STD.NO.=SIO2        0.        0.     30149.    14419.   900033.   141710.  1669800.    39231.
STD.NO.=BCS-309  1245.     4218.     10526.    14864.   602051.    94525.  1092687.    48222.
STD.NO.=BCS-367  2916.     4340.     10586.    14609.   634876.    88033.  1138797.    46549.
STD.NO.=BR       2290.     4624.     10302.    14716.   623955.    89826.  1110570.    47745.
STD.NO.=NBS-77   8804.     3474.     10501.    15029.   626567.    61537.  1108651.    45694.
STD.NO.=NIM-D    5536.     4659.      8514.    14690.   454095.    99029.  1186909.    48223.
STD.NO.=NIM-P    2690.     4708.     10535.    14717.   620207.    90933.  1031223.    48392.
STD.NO.=NIM-S    1482.     4700.     10368.    14611.   597959.    91251.  1252623.    47960.
STD.NO.=NS-1     2362.     4442.     10754.    14692.   616995.    86005.  1056243.    46681.
STD.NO.=SCH-1    9079.    17593.     11319.    15211.   782981.   165877.  1174236.    46307.

AVERAGE VALUES   4045.     5862.     12355.    14756.   645972.   100873.  1182174.    46500.

WHAT TYPE OF LSF CURVES DO YOU WANT TO USE FOR CALIBRATION :
  (1) Y=A0+A1*X      (2) Y=A0+A1*X+A2*X*X
  (3) Y=A1*X         (4) Y=A1*X+A2*X*X       ?  4
DO YOU WANT TO PRINT OUT LSF COEFFICIENTS (Y/N) :  Y

              TABULATION OF CALCULATED LSF COEFFICIENTS
                 (X=MEAS.INT.  ;  Y=CALC.REL.INT.)

NA2O      A0= 0.00000E+00  A1= 0.42687E-03  A2=-0.15095E-07
MGO       A0= 0.00000E+00  A1= 0.21600E-03  A2=-0.94955E-09
AL2O3     A0= 0.00000E+00  A1= 0.94525E-04  A2= 0.90422E-10
SIO2      A0= 0.00000E+00  A1= 0.66925E-04  A2= 0.16971E-09
K2O       A0= 0.00000E+00  A1= 0.15815E-05  A2= 0.10485E-11
CAO       A0= 0.00000E+00  A1= 0.10974E-04  A2= 0.13550E-10
TIO2      A0= 0.00000E+00  A1= 0.93351E-06  A2=-0.88733E-12
FE2O3     A0= 0.00000E+00  A1= 0.20589E-04  A2= 0.24027E-10

-----RESULTS OF LAST ITERATION-----


SMP.NO.=BX-N      R=NA2O     0.00043 MGO      0.00043 AL2O3    0.51756 SIO2     0.05963 K2O      0.00050 CAO      0.00184
                    TIO2     0.02919 FE2O3    0.29411
```

```
          L= 4  C=LOI      12.170% NA2O      0.049% MGO       0.048% AL2O3    55.088% SIO2     7.552% P2O5      0.130%
                  SO3       0.000% K2O       0.050% CAO       0.170% TIO2      2.300% CR2O3    0.000% MNO       0.050%
                  FE2O3    23.474%
                TOTAL= 101.08%

SMP.NO.=DT-N      R=NA2O    0.00000 MGO      0.00043 AL2O3    0.58246 SIO2     0.30159 K2O      0.00108 CAO      0.00042
                  TIO2      0.01622 FE2O3    0.00752
          L= 3  C=LOI       1.600% NA2O      0.000% MGO       0.044% AL2O3    58.403% SIO2    36.913% P2O5      0.090%
                  SO3       0.000% K2O       0.114% CAO       0.041% TIO2      1.363% CR2O3    0.040% MNO       0.010%
                  FE2O3     0.585%
                TOTAL=  99.19%

SMP.NO.=GH        R=NA2O    0.03660 MGO      0.00043 AL2O3    0.12550 SIO2     0.72149 K2O      0.04534 CAO      0.00707
                  TIO2      0.00091 FE2O3    0.01632
          L= 3  C=LOI       0.600% NA2O      3.888% MGO       0.045% AL2O3    12.810% SIO2    76.772% P2O5      0.010%
                  SO3       0.000% K2O       4.836% CAO       0.741% TIO2      0.081% CR2O3    0.000% MNO       0.050%
                  FE2O3     1.339%
                TOTAL= 101.17%

SMP.NO.=NBS-76    R=NA2O    0.00299 MGO      0.00562 AL2O3    0.37317 SIO2     0.48060 K2O      0.01470 CAO      0.00228
                  TIO2      0.02521 FE2O3    0.02697
          L= 3  C=LOI       0.220% NA2O      0.318% MGO       0.578% AL2O3    37.859% SIO2    55.540% P2O5      0.070%
                  SO3       0.000% K2O       1.560% CAO       0.230% TIO2      2.176% CR2O3    0.000% MNO       0.000%
                  FE2O3     2.180%
                TOTAL= 100.74%

SMP.NO.=NBS-99A   R=NA2O    0.06285 MGO      0.00043 AL2O3    0.20365 SIO2     0.59886 K2O      0.05072 CAO      0.02044
                  TIO2      0.00012 FE2O3    0.00093
          L= 3  C=LOI       0.260% NA2O      6.633% MGO       0.045% AL2O3    20.881% SIO2    65.851% P2O5      0.020%
                  SO3       0.000% K2O       5.376% CAO       2.145% TIO2      0.011% CR2O3    0.000% MNO       0.000%
                  FE2O3     0.077%
                TOTAL= 101.30%
```


TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	LOI	NA2O	MGO	AL2O3	SIO2	P2O5	SO3	K2O	CAO	TIO2	CR2O3	MNO	FE2O3
BX-N	101.08	12.170	0.049	0.048	55.088	7.552	0.130	0.000	0.050	0.170	2.300	0.000	0.050	23.474
DT-N	99.19	1.600	0.000	0.044	58.403	36.913	0.090	0.000	0.114	0.041	1.363	0.040	0.010	0.585
GH	101.17	0.600	3.888	0.045	12.810	76.772	0.010	0.000	4.836	0.741	0.081	0.000	0.050	1.339
NBS-76	100.74	0.220	0.318	0.578	37.859	55.540	0.070	0.000	1.560	0.230	2.176	0.000	0.000	2.180
NBS-99A	101.30	0.260	6.633	0.045	20.881	65.851	0.020	0.000	5.376	2.145	0.011	0.000	0.000	0.077

```
DO YOU WISH TO COMPARE THESE RESULTS WITH OTHER PREVIOUSLY KNOWN VALUES FOR THESE SPECIMENS (Y/N) ?  Y
ENTER KNOWN CONCENTRATIONS OF SPECIMENS :

SMP.NO.=BX-N       .1217,.0006,.0011,.5353,.0730,.0013,0.0,.0007,.0017,.0241,0.0,.0005,.2327
SMP.NO.=DT-N       .0160,.0004,.0004,.5921,.3652,.0009,0.0,.0012,.0004,.0140,.0004,.0001,.0066
SMP.NO.=GH         .0060,.0385,.0003,.1251,.7585,.0001,0.0,.0476,.0069,.0008,0.0,.0005,.0135
SMP.NO.=NBS-76     .0022,.0015,.0059,.3767,.5468,.0007,0.0,.0137,.0027,.0221,0.0,0.0,.0238
SMP.NO.=NBS-99A    .0026,.0620,.0002,.2050,.6520,.0002,0.0,.0520,.0214,.0001,0.0,0.0,.0006
```

TABULATION OF RESULTS (%)

SMP.NO.	TOTAL	LOI	NA2O	MGO	AL2O3	SIO2	P2O5	SO3	K2O	CAO	TIO2	CR2O3	MNO	FE2O3
BX-N	99.27	12.17	0.06	0.11	53.53	7.30	0.13	0.00	0.07	0.17	2.41	0.00	0.05	23.27
	101.08	12.17	0.05	0.05	55.09	7.55	0.13	0.00	0.05	0.17	2.30	0.00	0.05	23.47
	ABS.ERR.	0.00	-0.01	-0.06	1.56	0.25	0.00	0.00	-0.02	0.00	-0.11	0.00	0.00	0.20
	REL.ERR.	0.00	-16.67	-54.55	2.91	3.42	0.00	0.00	-28.57	0.00	-4.56	0.00	0.00	0.86
DT-N	99.77	1.60	0.04	0.04	59.21	36.52	0.09	0.00	0.12	0.04	1.40	0.04	0.01	0.66
	99.19	1.60	0.00	0.04	58.40	36.91	0.09	0.00	0.11	0.04	1.36	0.04	0.01	0.59
	ABS.ERR.	0.00	-0.04	0.00	-0.81	0.39	0.00	0.00	-0.01	0.00	-0.04	0.00	0.00	-0.07
	REL.ERR.	0.00	-100.00	0.00	-1.37	1.07	0.00	0.00	-8.33	0.00	-2.86	0.00	0.00	-10.61
GH	99.78	0.60	3.85	0.03	12.51	75.85	0.01	0.00	4.76	0.69	0.08	0.00	0.05	1.35
	101.17	0.60	3.89	0.04	12.81	76.77	0.01	0.00	4.84	0.74	0.08	0.00	0.05	1.34
	ABS.ERR.	0.00	0.04	0.01	0.30	0.92	0.00	0.00	0.08	0.05	0.00	0.00	0.00	-0.01
	REL.ERR.	0.00	1.04	33.33	2.40	1.21	0.00	0.00	1.68	7.25	0.00	0.00	0.00	-0.74
NBS-76	99.61	0.22	0.15	0.59	37.67	54.68	0.07	0.00	1.37	0.27	2.21	0.00	0.00	2.38
	100.74	0.22	0.32	0.58	37.86	55.54	0.07	0.00	1.56	0.23	2.18	0.00	0.00	2.18
	ABS.ERR.	0.00	0.17	-0.01	0.19	0.86	0.00	0.00	0.19	-0.04	-0.03	0.00	0.00	-0.20
	REL.ERR.	0.00	113.33	-1.69	0.50	1.57	0.00	0.00	13.87	-14.81	-1.36	0.00	0.00	-8.40
NBS-99A	99.61	0.26	6.20	0.02	20.50	65.20	0.02	0.00	5.20	2.14	0.01	0.00	0.00	0.06
	101.30	0.26	6.63	0.05	20.88	65.85	0.02	0.00	5.38	2.14	0.01	0.00	0.00	0.08
	ABS.ERR.	0.00	0.43	0.03	0.38	0.65	0.00	0.00	0.18	0.00	0.00	0.00	0.00	0.02
	REL.ERR.	0.00	6.94	150.00	1.85	1.00	0.00	0.00	3.46	0.00	0.00	0.00	0.00	33.33
AVG.ABS.ERR.		0.00	0.14	0.02	0.65	0.61	0.00	0.00	0.10	0.02	0.04	0.00	0.00	0.10
AVG.REL.ERR.		0.00	47.59	47.91	1.81	1.66	0.00	0.00	11.18	4.41	1.76	0.00	0.00	10.79

DO YOU WANT TO TRY ANOTHER TYPE OF CALIBRATION CURVE (Y/N) ? N

TTO -- STOP

Appendix 4: Listing of Programs for Creating and Reading Permanent Datafiles

```
      PROGRAM CREMAC
C
C       THIS PROGRAM CREATES A DATAFILE NAMED 'MACPRM.DAT'
C      FOR SAVING PARAMETERS NEEDED FOR CALCULATING MASS
C      ABSORPTION COEFFICIENTS WITH LEROUX ALGORITHM.
C      (1979 VERSION)
C
C       NBS        06-SEP-1984
C
      IMPLICIT INTEGER (I,J)
      IMPLICIT REAL (A-H,K-Z)
      OPEN (UNIT=3,NAME='MACPRM.DAT',TYPE='NEW',ACCESS='DIRECT',
     1 MAXREC=94,RECORDSIZE=24)
      DO 50 I=1,94
       WRITE(6,100)I
       READ(5,*)C,K,NK,EP,CK1,NCK1,L1,NL1,L2,NL2,L3,NL3,
     1  M1,NM1,M2,NM2,M3,NM3,M4,NM4,M5,NM5,N1,NN1
       WRITE(3'I) C,K,NK,EP,CK1,NCK1,L1,NL1,L2,NL2,L3,NL3,M1,NM1,M2,
     1  NM2,M3,NM3,M4,NM4,M5,NM5,N1,NN1
50    CONTINUE
      CLOSE (UNIT=3)
100   FORMAT(' Z=',I3)
      END


      PROGRAM RDCREMAC
C
C      THIS PROGRAM PRINTS OUT THE CONTENTS OF THE
C      DATAFILE NAMED 'MACPRM.DAT'.
C
C      NBS        06-SEP-1984
C
      IMPLICIT INTEGER (I,J)
      IMPLICIT REAL (A-H,K-Z)
      OPEN (UNIT=3,NAME='MACPRM.DAT',TYPE='OLD',ACCESS='DIRECT',
     1  MAXREC=94,RECORDSIZE=24)
      DO 10 I=1,94
      READ(3'I) C,K,NK,EP,CK1,NCK1,L1,NL1,L2,NL2,L3,NL3,M1,NM1,
     1  M2,NM2,M3,NM3,M4,NM4,M5,NM5,N1,NN1
      WRITE(6,100) C,K,NK,EP,CK1,NCK1,L1,NL1,L2,NL2,L3,NL3,M1,NM1,
     1  M2,NM2,M3,NM3,M4,NM4,M5,NM5,N1,NN1
10    CONTINUE
      CLOSE(UNIT=3)
      STOP
100   FORMAT(/1X,12F9.4)
      END
```

```
      PROGRAM WRITTGT
C
C     THIS PROGRAM WRITES A DIRECT DATAFILE CALLED
C     'TGTWR.DAT' TO PROVIDE INFORMATION NEEDED FOR
C     CALCULATING CHARACTERISTIC LINE INTENSITIES
C     IN AN X-RAY TUBE SPECTRUM.
C
C     NBS        06-SEP-1984
C
      DIMENSION DAT(14,11)
      OPEN(UNIT=3,NAME='TGTWR.DAT',TYPE='NEW',ACCESS='DIRECT',
     +  MAXREC=14,RECORDSIZE=11)
      WRITE(6,5)
5     FORMAT(1X,'INPUT DATA BY KEYBOARD:'/)
      DO 10 I=1,14
      READ(5,*)(DAT(I,J),J=1,11)
      WRITE(3'I)(DAT(I,J),J=1,11)
10    CONTINUE
      CLOSE(UNIT=3)
      END



PROGRAM RDWRTTGT
C
C     THIS PROGRAM PRINTS OUT THE CONTENTS OF
C     DATAFILE NAMED 'TGTWR.DAT'.
C
C     NBS        06-SEP-1984
C
      DIMENSION DAT(14,11)
      OPEN(UNIT=3,NAME='TGTWR.DAT',TYPE='OLD',ACCESS='DIRECT',
     +  MAXREC=14,RECORDSIZE=11)
      DO 20 I=1,14
      READ(3'I)(DAT(I,J),J=1,11)
      WRITE(6,100)(DAT(I,J),J=1,11)
20    CONTINUE
      CLOSE(UNIT=3)
100   FORMAT(/1X,11(F8.4,2X))
      END
```

Contents of the permanent datafile called 'MACPRM.DAT' for calculating mass absorption coefficients using the expression of Thinh and Leroux. The following tabulated values are in the same order as given in Table 1 of reference 10.

0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.0727	0.0246	3.0300	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.8894	0.0548	3.0300	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.4604	0.1110	3.0300	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.0824	0.1880	3.0300	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.8531	0.2838	3.0940	1.7500	2.1900	2.7345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.5355	0.4016	3.0660	2.1200	3.2600	2.7345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.3268	0.5320	3.0410	2.5000	4.6100	2.7345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.1058	0.6854	3.0190	3.0000	6.2500	2.7345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.8419	0.8669	3.0000	3.5500	8.2000	2.7345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.5844	1.0721	2.9830	4.4000	10.4900	2.7345	0.0633	2.8350	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.3105	1.3050	2.9670	6.4000	13.1400	2.7345	0.0894	2.8200	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.5946	1.5596	2.9530	6.2000	16.1600	2.7345	0.1177	2.8050	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.1309	1.8389	2.9400	5.9000	19.5700	2.7345	0.1487	2.7900	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.6522	2.1455	2.9270	6.7000	23.3900	2.7345	0.1893	2.7750	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.1931	2.4720	2.9160	7.5000	27.6300	2.7345	0.2292	2.7600	0.0000	0.0000	0.0000	0.0000

Values - Continued

0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.7343	2.8224	2.9050	8.4000	32.3200	2.7345	0.2702	2.7450	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.2540	3.2029	2.8950	9.5000	37.4700	2.7345	0.3200	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.7770	3.6074	2.8860	11.0900	43.0800	2.7345	0.3771	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.2904	4.0381	2.8500	13.3000	49.1900	2.7345	0.4378	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.5125	4.4928	2.8500	13.2000	55.8000	2.7345	0.5004	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.7473	4.9664	2.8500	13.0000	62.9300	2.7345	0.5637	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.9768	5.4651	2.8500	12.9500	70.5900	2.7345	0.6282	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.2009	5.9892	2.8500	12.9000	78.7900	2.7345	0.6946	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.4196	6.5390	2.8500	12.6000	87.5600	2.7345	0.7690	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.6384	7.1120	2.8500	12.5000	96.8900	2.7345	0.8461	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.8555	7.7089	2.8500	12.4000	106.8200	2.7345	0.9256	2.7300	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.0657	8.3328	2.8500	12.4000	117.3400	2.7345	1.0081	2.7300	0.8719	2.6144	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.2775	8.9789	2.8500	12.1000	128.4800	2.7345	1.0961	2.7300	0.9510	2.6144	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.4732	9.6586	2.8500	12.0000	140.2500	2.7345	1.1936	2.7300	1.0428	2.6144	1.0197	2.3554
0.1359	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.6620	10.3671	2.8500	12.0000	152.6500	2.7345	1.2977	2.7300	1.1423	2.6144	1.1154	2.3554
0.1581	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.8464	11.1031	2.8500	12.0000	165.7000	2.7345	1.4143	2.7300	1.2478	2.6144	1.2167	2.3554

Values - Continued

0.1800	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.0268	11.8667	2.8500	12.0000	179.4100	2.7345	1.5265	2.7300	1.3586	2.6144	1.3231	2.3554
0.2035	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.2038	12.6578	2.8500	0.0000	0.0000	0.0000	1.6539	2.7300	1.4762	2.6144	1.4358	2.3554
0.2315	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.3807	13.4737	2.8500	0.0000	0.0000	0.0000	1.7820	2.7300	1.5960	2.6144	1.5499	2.3554
0.2565	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.5452	14.3256	2.8500	0.0000	0.0000	0.0000	1.9210	2.7300	1.7272	2.6144	1.6749	2.3554
0.2850	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.7132	15.1997	2.8500	0.0000	0.0000	0.0000	2.0651	2.7300	1.8639	2.6144	1.8044	2.3554
0.3221	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.8756	16.1046	2.8500	0.0000	0.0000	0.0000	2.2163	2.7300	2.0068	2.6144	1.9396	2.3554
0.3575	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.0348	17.0384	2.8500	0.0000	0.0000	0.0000	2.3725	2.7300	2.1555	2.6144	2.0800	2.3554
0.3936	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.1942	17.9976	2.8500	0.0000	0.0000	0.0000	2.5316	2.7300	2.3067	2.6144	2.2223	2.3554
0.4303	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.3507	18.9856	2.8500	0.0000	0.0000	0.0000	2.6977	2.7300	2.4647	2.6144	2.3705	2.3554
0.4684	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.5071	19.9995	2.8500	0.0000	0.0000	0.0000	2.8655	2.7300	2.6251	2.6144	2.5202	2.3554
0.5046	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.6595	21.0440	2.8500	0.0000	0.0000	0.0000	3.0425	2.7300	2.7932	2.6144	2.6769	2.3554
0.5400	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.8097	22.1172	2.8500	0.0000	0.0000	0.0000	3.2240	2.7300	2.9669	2.6144	2.8379	2.3554
0.5850	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.9573	23.2199	2.8500	0.0000	0.0000	0.0000	3.4119	2.7300	3.1461	2.6144	3.0038	2.3554
0.6271	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.1037	24.3503	2.8500	0.0000	0.0000	0.0000	3.6043	2.7220	3.3303	2.6144	3.1733	2.3554
0.6699	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.2453	25.5140	2.8500	0.0000	0.0000	0.0000	3.8058	2.7140	3.5237	2.6144	3.3511	2.3554
0.7175	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.3824	26.7112	2.8500	0.0000	0.0000	0.0000	4.0180	2.7060	3.7270	2.6144	3.5375	2.3554

Values - Continued

0.7702	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.5165	27.9399	2.8500	0.0000	0.0000	0.0000	4.2375	2.6980	3.9380	2.6144	3.7301	2.3554
0.8256	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.6481	29.2001	2.8500	0.0000	0.0000	0.0000	4.4647	2.6900	4.1561	2.6144	3.9288	2.3554
0.8838	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.7775	30.4912	2.8500	0.0000	0.0000	0.0000	4.6983	2.6820	4.3804	2.6144	4.1322	2.3554
0.9437	2.6000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.9048	31.8138	2.8500	0.0000	0.0000	0.0000	4.9392	2.6740	4.6120	2.6144	4.3414	2.3554
1.0060	2.6000	0.8697	2.4471	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.0291	33.1694	2.8500	0.0000	0.0000	0.0000	5.1881	2.6660	4.8521	2.6144	4.5571	2.3554
1.0721	2.6000	0.9305	2.4471	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.1326	34.5614	2.8500	0.0000	0.0000	0.0000	5.4528	2.6580	5.1037	2.6144	4.7822	2.3554
1.1400	2.6000	0.9990	2.4471	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.2062	35.9846	2.8500	0.0000	0.0000	0.0000	5.7143	2.6500	5.3594	2.6144	5.0119	2.3554
1.2171	2.6000	1.0650	2.4471	0.9976	2.4471	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.2781	37.4406	2.8500	0.0000	0.0000	0.0000	5.9888	2.6500	5.6236	2.6144	5.2470	2.3554
1.2928	2.6000	1.1367	2.4471	1.0622	2.4471	0.7961	2.4000	0.0000	0.0000	0.0000	0.0000
18.3506	38.9246	2.8500	0.0000	0.0000	0.0000	6.2663	2.6500	5.8906	2.6144	5.4827	2.3554
1.3613	2.6000	1.2044	2.4471	1.1234	2.4471	0.8485	2.4000	0.0000	0.0000	0.0000	0.0000
18.4209	40.4430	0.0000	0.0000	0.0000	0.0000	6.5488	2.6500	6.1642	2.6144	5.7234	2.3554
1.4346	2.6000	1.2728	2.4471	1.1854	2.4471	0.9013	2.4000	0.0000	0.0000	0.0000	0.0000
18.4913	41.9906	0.0000	0.0000	0.0000	0.0000	6.8348	2.6500	6.4404	2.6144	5.9643	2.3554
1.5110	2.6000	1.3374	2.4471	1.2422	2.4471	0.9511	2.4000	0.0000	0.0000	0.0000	0.0000
18.5613	43.5689	0.0000	0.0000	0.0000	0.0000	7.1260	2.6500	6.7215	2.6144	6.2079	2.3554
1.5753	2.6000	1.4028	2.4471	1.2974	2.4471	0.9999	2.4000	0.0000	0.0000	0.0000	0.0000
18.6282	45.1840	0.0000	0.0000	0.0000	0.0000	7.4279	2.6500	7.0128	2.6144	6.4593	2.3554
1.6540	2.5750	1.4714	2.4471	1.3569	2.4471	1.0515	2.4000	1.0269	2.2000	0.3300	2.4980
18.6932	46.8342	0.0000	0.0000	0.0000	0.0000	7.7368	2.6500	7.3118	2.6144	6.7162	2.3554
1.7228	2.5750	1.5407	2.4471	1.4198	2.4471	1.1060	2.4000	1.0802	2.2000	0.3457	2.4920
18.7564	48.5190	0.0000	0.0000	0.0000	0.0000	8.0520	2.6500	7.6171	2.6144	6.9769	2.3554
1.8000	2.5750	1.6139	2.4471	1.4806	2.4471	1.1606	2.4000	1.1309	2.2000	0.3602	2.4850
18.8179	50.2391	0.0000	0.0000	0.0000	0.0000	8.3756	2.6500	7.9303	2.6144	7.2428	2.3554

Values - Continued

1.8808	2.5750	1.6883	2.4471	1.5440	2.4471	1.2172	2.4000	1.1852	2.2000	0.3758	2.4790
18.8773	51.9957	0.0000	0.0000	0.0000	0.0000	8.7080	2.6500	8.2516	2.6144	7.5140	2.3554
1.9675	2.5750	1.7677	2.4471	1.6113	2.4471	1.2750	2.4000	1.2412	2.2000	0.3979	2.4720
18.9350	53.7885	0.0000	0.0000	0.0000	0.0000	9.0458	2.6500	8.5806	2.6144	7.7901	2.3554
2.0468	2.5750	1.8418	2.4471	1.6756	2.4471	1.3325	2.4000	1.2949	2.2000	0.4163	2.4660
18.9909	55.6177	0.0000	0.0000	0.0000	0.0000	9.3942	2.6500	8.9178	2.6144	8.0711	2.3554
2.1283	2.5750	1.9228	2.4471	1.7412	2.4471	1.3915	2.4000	1.3514	2.2000	0.4357	2.4600
19.0446	57.4855	0.0000	0.0000	0.0000	0.0000	9.7513	2.6500	9.2643	2.6144	8.3579	2.3554
2.2065	2.5750	2.0058	2.4471	1.8118	2.4471	1.4533	2.4000	1.4093	2.2000	0.4491	2.4540
19.0969	59.3896	0.0000	0.0000	0.0000	0.0000	10.1157	2.6500	9.6169	2.6144	8.6480	2.3554
2.3068	2.5750	2.0898	2.4471	1.8845	2.4471	1.5146	2.4000	1.4677	2.2000	0.4717	2.4480
19.1472	61.3323	0.0000	0.0000	0.0000	0.0000	10.4864	2.6500	9.9782	2.6144	8.9436	2.3554
2.3981	2.5750	2.1730	2.4471	1.9498	2.4471	1.5763	2.4000	1.5278	2.2000	0.4872	2.4420
19.1957	63.3138	0.0000	0.0000	0.0000	0.0000	10.8704	2.6500	10.3486	2.6144	9.2441	2.3554
2.4912	2.5750	2.2635	2.4471	2.0236	2.4471	1.6394	2.4000	1.5885	2.2000	0.5062	2.4360
19.2376	65.3508	0.0000	0.0000	0.0000	0.0000	11.2707	2.6500	10.7394	2.6144	9.5607	2.3554
2.6009	2.5750	2.3654	2.4471	2.1076	2.4471	1.7164	2.4000	1.6617	2.2000	0.5381	2.4300
19.2812	67.4164	0.0000	0.0000	0.0000	0.0000	11.6815	2.6500	11.1361	2.6144	9.8811	2.3554
2.7080	2.5750	2.4687	2.4471	2.1940	2.4471	1.7932	2.4000	1.7351	2.2000	0.5655	2.4250
19.3223	69.5250	0.0000	0.0000	0.0000	0.0000	12.0998	2.6500	11.5440	2.6144	10.2068	2.3554
2.8196	2.5750	2.5749	2.4471	2.2810	2.4471	1.8716	2.4000	1.8092	2.2000	0.5950	2.4190
19.3611	71.6764	0.0000	0.0000	0.0000	0.0000	12.5267	2.6500	11.9587	2.6144	10.5353	2.3554
2.9317	2.5750	2.6818	2.4471	2.3673	2.4471	1.9489	2.4000	1.8829	2.2000	0.6250	2.4140
19.3979	73.8706	0.0000	0.0000	0.0000	0.0000	12.9680	2.6500	12.3850	2.6144	10.8709	2.3554
3.0485	2.5750	2.7922	2.4471	2.4572	2.4471	2.0308	2.4000	1.9601	2.2000	0.6543	2.4080
19.4320	76.1110	0.0000	0.0000	0.0000	0.0000	13.4185	2.6500	12.8241	2.6144	11.2152	2.3554
3.1737	2.5750	2.9087	2.4471	2.5507	2.4471	2.1161	2.4000	2.0404	2.2000	0.6901	2.4030
19.4643	78.3948	0.0000	0.0000	0.0000	0.0000	13.8799	2.6500	13.2726	2.6144	11.5637	2.3554
3.2960	2.5750	3.0265	2.4471	2.6454	2.4471	2.2019	2.4000	2.1216	2.2000	0.7220	2.3980
19.4943	80.7249	0.0000	0.0000	0.0000	0.0000	14.3528	2.6500	13.7336	2.6144	11.9187	2.3554
3.4249	2.5750	3.1478	2.4471	2.7430	2.4471	2.2911	2.4000	2.2057	2.2000	0.7588	2.3930
19.5219	83.1023	0.0000	0.0000	0.0000	0.0000	14.8393	2.6500	14.2087	2.6144	12.2839	2.3554

Values - Continued

3.5616	2.5750	3.2785	2.4471	2.8471	2.4471	2.3849	2.4000	2.2949	2.2000	0.8003	2.3880
19.5466	85.5304	0.0000	0.0000	0.0000	0.0000	15.3467	2.6500	14.6979	2.6144	12.6575	2.3554
3.7041	2.5750	3.4157	2.4471	2.9566	2.4471	2.4851	2.4000	2.3893	2.2000	0.8455	2.3830
19.5696	88.0045	0.0000	0.0000	0.0000	0.0000	15.8608	2.6500	15.2000	2.6144	13.0352	2.3554
3.8507	2.5750	3.5542	2.4471	3.0664	2.4471	2.5856	2.4000	2.4840	2.2000	0.8936	2.3780
19.5909	90.5259	0.0000	0.0000	0.0000	0.0000	16.3875	2.6500	15.7111	2.6144	13.4186	2.3554
3.9991	2.5750	3.6963	2.4471	3.1769	2.4471	2.6876	2.4000	2.5796	2.2000	0.9382	2.3730
19.6083	93.1050	0.0000	0.0000	0.0000	0.0000	16.9393	2.6500	16.2443	2.6144	13.8138	2.3554
4.1494	2.5750	3.8541	2.4471	3.3019	2.4471	2.7980	2.4000	2.6830	2.2000	0.9953	2.3680
19.6248	95.7299	0.0000	0.0000	0.0000	0.0000	17.4930	2.6500	16.7847	2.6144	14.2135	2.3554
4.3170	2.5750	4.0080	2.4471	3.4260	2.4471	2.9087	2.4000	2.7867	2.2000	1.0420	2.3640
19.6395	98.4040	0.0000	0.0000	0.0000	0.0000	18.0490	2.6500	17.3371	2.6144	14.6194	2.3554
4.4820	2.5750	4.1590	2.4471	3.5380	2.4471	3.0215	2.4000	2.8924	2.2000	1.0970	2.3590
19.6510	101.1370	0.0000	0.0000	0.0000	0.0000	18.6390	2.6500	17.9065	2.6144	15.0312	2.3554
4.6520	2.5750	4.3270	2.4471	3.6630	2.4471	3.1362	2.4000	2.9999	2.2000	1.1530	2.3550
19.6607	103.9219	0.0000	0.0000	0.0000	0.0000	19.2367	2.6500	18.4843	2.6144	15.4444	2.3554
4.8220	2.5750	4.4895	2.4471	3.7918	2.4471	3.2484	2.4000	3.1049	2.2000	1.2084	2.3500
19.6695	106.7553	0.0000	0.0000	0.0000	0.0000	19.8400	2.6500	19.0832	2.6144	15.8710	2.3554
5.0020	2.5750	4.6560	2.4471	3.9090	2.4471	3.3702	2.4000	3.2190	2.2000	1.2690	2.3460
19.6749	109.6509	0.0000	0.0000	0.0000	0.0000	20.4721	2.6500	19.6932	2.6144	16.3003	2.3554
5.1823	2.5750	4.8304	2.4471	4.0461	2.4471	3.4908	2.4000	3.3320	2.2000	1.3295	2.3410
19.6786	112.6014	0.0000	0.0000	0.0000	0.0000	21.1046	2.6500	20.3137	2.6144	16.7331	2.3554
5.3669	2.5750	5.0009	2.4471	4.1738	2.4471	3.6112	2.4000	3.4418	2.2000	1.3871	2.3370
19.6808	115.6061	0.0000	0.0000	0.0000	0.0000	21.7574	2.6500	20.9476	2.6144	17.1663	2.3554
5.5480	2.5750	5.1822	2.4471	4.3034	2.4471	3.7276	2.4000	3.5517	2.2000	1.4408	2.3330
19.6796	118.6780	0.0000	0.0000	0.0000	0.0000	22.4268	2.6500	21.6005	2.6144	17.6100	2.3554
5.7232	2.5750	5.3662	2.4471	4.4347	2.4471	3.8503	2.4000	3.6658	2.2000	1.5007	2.3280
19.6751	121.8180	0.0000	0.0000	0.0000	0.0000	23.0972	2.6500	22.2662	2.6144	18.0568	2.3554
5.9329	2.5750	5.5412	2.4471	4.5566	2.4471	3.9726	2.4000	3.7781	2.2000	1.5586	2.3240

Contents of the Permanent Datafile Called 'TGTWR.DAT'

3.0320	2.7800	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.2910	2.0850	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.7100	0.6320	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.6140	0.5460	4.5970	4.3740	4.1300	4.2530	4.2890	3.9440	0.0000	0.0000	0.0000
0.0000	0.0000	1.0000	0.5400	0.1150	0.1070	0.0700	0.0680	0.0000	0.0000	0.0000
0.5610	0.4970	4.1540	3.9350	3.7030	3.8340	3.8700	3.5230	0.0000	0.0000	0.0000
0.0000	0.0000	1.0000	0.5270	0.1880	0.0840	0.0520	0.1070	0.0000	0.0000	0.0000
0.0000	0.0000	1.4760	1.2820	1.2450	1.2630	1.3020	1.0980	1.0680	1.0620	1.6780
0.0000	0.0000	1.0000	0.4660	0.1790	0.0740	0.0470	0.0810	0.0130	0.0180	0.0290
0.0000	0.0000	1.2770	1.0830	1.0700	1.0680	1.1060	0.9270	0.9050	0.8980	1.4600
0.0000	0.0000	1.0000	0.4580	0.2060	0.0740	0.0470	0.0990	0.0100	0.0200	0.0310

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NBSGSC--A FORTRAN Program for Quantitative X-ray Fluorescence Analysis

5. AUTHOR(S)

G. Y. Tao, P. A. Pella, and R. M. Rousseau

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

NATIONAL BUREAU OF STANDARDS
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8. Type of Report & Period Covered

Final

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

Same as in item 6 above.

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 program (NBSGSC) was developed for performing quantitative analysis of bulk specimens by x-ray fluorescence spectrometry. This program corrects for x-ray absorption/enhancement phenomena using the comprehensive alpha coefficient algorithm proposed by Lachance (COLA). NBSGSC is a revision of the program ALPHA and CARECAL originally developed by R.M. Rousseau of the Geological Survey of Canada. Part one of the program (CALCO) performs the calculation of theoretical alpha coefficients, and part two (CALCOMP) computes the composition of the analyte specimens. The analysis of alloys, pressed minerals, and fused specimens can currently be treated by the program. In addition to using measured x-ray tube spectral distributions, spectra from seven commonly used x-ray tube targets could also be calculated with an NBS algorithm included in the program. NBSGSC is written in FORTRAN IV for a Digital Equipment Corporation (DEC PDP-11/23) minicomputer using RL02 firm disks and an RSX 11M operating system.

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

alpha coefficients; comprehensive algorithm; fundamental parameters; interelement corrections; program; quantitative analysis; x-ray.

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