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A COMPUTER PROGRAM FOR ELECTRON PROBE MICROANALYSIS IN THE FIELDS OF METALLURGY AND GEOLOGY

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GODDARD SPACE FLIGHT CENTER
GREENBELT, MARYLAND

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ABSTRACT

A comprehensive computer program has been written which should prove useful to investigators in both the fields of metallurgy and geology. The program is flexible in both input and output and is relatively easy for an inexperienced person to use. It is written in the Fortran language and can be used in remote terminal operation which is now available in many laboratories. The program is built up of a large number of subroutines which can be easily changed as the user sees fit or as new correction schemes become available. At present, the following corrections are incorporated; the absorption correction of Philibert-Duncumb [1,2] recently modified by Heinrich,[3] the atomic number correction of Duncumb and Reed,[4] and the fluorescence correction of Reed.[5] K_α x-ray radiation from elements of atomic numbers 3-39 and L_α radiation from elements of atomic numbers 20-92 are considered. The program operates in either of two modes; conversion of raw intensity data to composition using an iterative procedure, or conversion of compositional data to expected x-ray intensities. For problems in geology involving oxides, calculations are made with oxygen considered as a matrix element. Specimens and complex standards each containing up to nine elements can be treated and several standards can be used for each element measured in order to check the consistency of the answer. The program determines internally whether a fluorescence correction is necessary and also calculates the initial intensity ratios. The program does not correct for non-normal incidence or continuum excitation. An exhaustive print out of the various correction factors can be obtained if desired.

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The program is rather unique with respect to the method of data handling and ease of operation. All the critical data for a given element, such as x-ray wave lengths, fluorescence yields, atomic weights, absorption edge jump ratios and the necessary factors for the calculation of mass absorption coefficients from Heinrich [6] are stored on cards or are placed on file at the computer. These data are then used as needed for the elements under consideration in each problem. The compositional data for each of the element standards are also stored on cards or at the computer. The input data which specifies the problem of interest then requires a minimum of information and can be supplied in a non-rigid format.

A COMPUTER PROGRAM FOR ELECTRON MICROPROBE ANALYSIS IN THE FIELDS OF METALLURGY AND GEOLOGY

I. INTRODUCTION

The electron microprobe has been used to solve problems in many fields of scientific research such as metallurgy, geology and biology. In the area of quantitative microchemistry the results of microprobe analysis have not fully met the expectations of the early pioneers. Schemes which correct the x-ray data for the effect of atomic number, absorption and fluorescence have been used extensively. However at this time precision errors (Ziebold)[7] and errors in the input parameters to the various correction schemes (Heinrich and Yakowitz)[8] limit the precision and accuracy of the analysis to no better than about 2% relative. Comparisons between measured intensity data from well characterized standards and calculated intensity ratios (Ziebold and Ogilvie,[9] Goldstein, et al.[10] and Beaman[11]) support this conclusion.

To avoid using any corrections for microprobe analysis, standard samples with similar compositions to the analyzed sample must be obtained. In the vast majority of cases this is not practical, and the correction schemes must be used. As the number of unknown elements, standard samples and data points desired increases, the amount of data handling and calculation becomes excessive. The use of computer techniques allows rapid handling of data, accurate calculation of correction procedures and assimilation of output in a useful form. With the development of remote terminal operation and rapid microprobe readout devices, the need for computer programs for quantitative electron microprobe analysis has developed.

About 20 computer programs for electron probe microanalysis are now available. Descriptions of the various programs are presently being compiled by Beaman[12] and need not be discussed here. In general many of these programs are either inflexible, are written for specific computer systems or are only able to handle a small number of elements or standards. Since problems originating in various disciplines are often run in the same microprobe facility, a program was designed that could be used to treat both geologic and metallurgical problems. We desired a flexible program built on a modular design with minimal input and data handling, compatible with remote terminal operation, and incorporating the best correction procedures currently available.

This paper describes the program we have developed. The program design, calculation schemes and input-output are described in sufficient detail so that the computer program can be adopted for use in most laboratories. Several sample problems are discussed in order to illustrate the use of the program.

II. CORRECTION PROCEDURES FOR ELECTRON MICROPROBE ANALYSIS

A. Corrections to Raw Intensity Data

To obtain an analysis for each element in a sample of interest the following measurements are made: (1) the x-ray intensity from the element standard taken both before and after the analysis, (2) the x-ray intensity from the background standard or the continuum radiation above and below the x-ray peak, and (3) the x-ray intensity for each element from the sample of interest. Three changes are made in the raw data, so that it is in a suitable form for calculations of the x-ray corrections.

1. Detector Dead Time – Detector dead-time causes a discrepancy between the true count rate of x-rays incident on a detector and the measured count rate. This relation is expressed as:

$$N = n/(1 - n\tau) \qquad (1)$$

where N is the true count rate, n is the measured count rate and τ is the detector dead time. This correction is applied separately for each element.

2. Drift – Drift is the slow change in x-ray signal caused by instabilities in the electronic system of the microanalyzer. Normally this change is less than 1% unless unusually long analysis times are used. In this program, if the standard intensity for each element differs, from the beginning to the end of an analysis, by more than 6 times the square root of the average standard intensity, a drift correction is applied. It has been found in practice that if the change in a monitored signal is no more than 5% per hour, then it may be assumed that the drift is linear in time. A linear drift correction is therefore applied when necessary.

3. Background – Background intensity arises from the continuous x-ray spectrum generated in the sample. It is obtained for each element by either measurement of the element intensity from a background standard or at spectrometer settings away from the Bragg angle. When samples of interest contain

many elements it is difficult to obtain an ideal background standard, that is, one which contains all the elements except the element being measured. Therefore the background is commonly measured by the second method. In the computer program, the background intensity is subtracted directly after the data is corrected for dead time.

B. Correction Procedures for the Conversion of X-Ray Intensity to Composition

It was first demonstrated by Castaing[13] that the relationship between the mass concentration, C_A, of an element, A, in a specimen analyzed in the microprobe and the ratio $(k_A = I_A/I(A))$ of the intensity of the characteristic x-ray line of element A measured from the specimen, I_A, to that measured from a standard, I(A), is, to a first approximation, linear:

$$k_A = C_A/C(A) \tag{2}$$

where C(A) is the amount of A present in the standard. If the standard consists of pure A, then

$$k_A = C_A. \tag{3}$$

Departures from the simple law of proportionality expressed in Equations 2, 3 can be large. Therefore if quantitative microchemical analysis is to be attempted with the microprobe, it is essential to apply a correction factor:

$$k_A = I_A/I(A) = \frac{C_A\ (\text{correction factor})_{\text{unknown}}}{C(A)\ (\text{correction factor})_{\text{std.}}} \tag{4}$$

This factor, is needed for the standard when it is not a pure element. The correction factor is placed on the right hand side of the equation because it is itself a function of C_A, C(A) and of the concentrations of the other elements present.

Following Castaing, most authors have divided the total correction into 3 separate factors: atomic number, absorption and fluorescence. The atomic number correction takes into account the effect of composition or atomic number on the intensity of characteristic x-rays generated within a specimen. The absorption correction allows for the absorption of characteristic x-rays in emerging from the specimen. The fluorescence correction allows for the additional intensity

contributed by fluorescence radiation which is due to excitation by x-rays from other elements in the specimen. The measured intensity ratio is therefore given by:

$$k_A = \frac{I_A}{I(A)} = \frac{C_A\,[At.\#]_u\,[Abs]_u\,[fluor]_u}{C(A)\,[At.\#]_s\,[Abs]_s\,[fluor]_s} \qquad (5)$$

where u represents the specimen of interest and s represents the standard. In most geologic problems C(A) is not equal to 1.0 and Equation 5 must be applied.

In the following sections the three corrections which are applied to unknown and standard intensities are described in detail. They were chosen as the best correction schemes available to date. It should be noted that none of these schemes correct for a non-normal electron beam. In the program the three correction schemes are incorporated in separate subroutines so that they can be easily changed if better corrections are developed.

1. Atomic Number Correction – The atomic number correction takes account of the fact that both the fraction of the total energy loss of an electron going into ionization of a particular shell (S) and the loss of ionization efficiency due to backscattering (R) are functions of atomic number. The atomic number correction is usually expressed as a ratio of backscattering to stopping power:

$$[At.\ No.]_u = [\bar{R}/\bar{S}]_u$$
$$[At.\ No.]_s = [\bar{R}/\bar{S}]_s \qquad (6)$$

Of the 3 major corrections, the atomic number correction appears to be the least developed. Uncertainties appear to lie in the accuracy of the R values available, in the validity of the Bethe equation for stopping power and in the value of J to be used in the Bethe stopping power. The correction according to Duncumb and Reed[4] provides a method for the correction that is easy to apply and appears to be achieving some acceptance. This formulation provides accuracies of the order of a few percent (Duncumb et al.).[14]

According to Duncumb-Reed,[4]

$$\bar{R} = \sum_i R_i\,C_i$$

for a complex sample where R_i is the backscatter coefficient for each element, C_i is the mass fraction of the i^{th} element and R_i is a function of 1/U, the reciprocal of the overvoltage. $\overline{S}$ may be obtained by using an expression of the form

$$\overline{S} = \sum_i C_i S_i$$

where:

$$S_i = Z_i/A_i \ln \left(\frac{1.166 \times 10^3 \overline{E}}{J_i}\right) \qquad (7)$$

and $\overline{E} = (E_0 - E_c)/2$ for each element in the sample. E_0 is the operating voltage and E_c is the excitation voltage of the x-ray line of interest. The mean ionization potential J_i was determined empirically as a function of atomic number Z.[4] The atomic number correction $\overline{R}/\overline{S}$ can therefore be calculated for both unknown and standard. It should be noted that the correction is the same for all the elements in the sample.

2. Absorption Correction – The absorption correction for both the analyzed sample and standard is given by the absorption function $f(\chi)$, where $[Abs]_u = f(\chi)_u$ and $[Abs]_s = f(\chi)_s$. The absorption correction procedure of Philibert[1] modified by Duncumb and Shields[2] is widely accepted as satisfactory, especially if $f(\chi)$ has a value between 0.3 and 1.0 (Yakowitz and Heinrich).[8]

The absorption function for each element analyzed in a sample is given by:

$$[Abs]_u = f(\chi)_u = 1 + h/\left((1 + \chi/\sigma)\ [1 + h\ (1 + \chi/\sigma)]_u\right), \qquad (8)$$

$$[Abs]_s = f(\chi)_s = 1 + h/\left((1 + \chi/\sigma)\ [1 + h\ (1 + \chi/\sigma)]_s\right)$$

in which

1. $\chi = (\mu/\rho)\ \csc\theta$ where μ/ρ is the mass absorption coefficient of the target for the measured x-ray line:

$$\mu/\rho = \sum_i C_i\ \mu/\rho_i \qquad (9)$$

and C_i = wt.% of element i
μ/ρ_i = mass absorption coefficient of element i for the x-ray line of interest.
θ = is the take-off angle of the emitted radiation.

2.

$$h = 1.2 \sum_i \alpha_i A_i / \left(\sum_i \alpha_i Z_i \right)^2 \qquad (10)$$

where α_i is the atomic concentration; A_i, the atomic weight; and Z_i, the atomic number of element i in the multi-element sample. The atomic concentration, α_i, is approximated by the weight fraction, C_i, within the program.

3.

$$\sigma = \frac{C \times 10^5}{E_0^n - E_c^n} \qquad (11)$$

where E_c is the excitation potential of the element of interest and E_0 is the electron beam operating voltage. Heinrich[3] proposed the values, C = 4.5 and n = 1.65. Recent studies by Duncumb, et al.[14] Show these values of C and n to be about optimum. The absorption function, $f(\chi)$, must be recalculated when another element is analyzed or when C_A changes. This correction limits the general applicability of the calculation procedure because μ/ρ values are not available for long wavelength L_α radiation.

3. Fluorescence Correction – The fluorescence correction for characteristic x-rays is required when one or more of the elements present in the specimen or standard has a characteristic emission line with energy greater than the critical excitation potential of the line being measured. In this case a fraction of the intensity observed, I_f/I_p, is due to fluorescence excitation rather than direct excitation. I_f represents the intensity due to fluorescence and I_p represents the primary intensity from the radiation of interest. The fluorescence correction for characteristic x-rays is given by:

$$[fluor]_u = \left[1 + \sum_i \frac{I_f}{I_p} \right]_u$$

$$[fluor]_s = \left[1 + \sum_i \frac{I_f}{I_p} \right]_s \qquad (12)$$

where I_f/I_p is summed over all the elements which cause fluorescence. The secondary fluorescence correction procedure developed by Castaing[13] and modified by Reed[5] has received the widest acceptance and seems to be the most suitable for general usage. The modified version of Castaing's correction formula for K - K fluorescence involving L lines is given by:

$$\left(\frac{I_f}{I_p}\right)_A = 0.5 P_{ij} C_B \left(\frac{r_A - 1}{r_A}\right) W(B) \frac{A}{B} \left(\frac{U_B - 1}{U_A - 1}\right)^{1.67} \frac{\mu_B^A}{\mu_B} \left(\frac{\ln(1+X)}{X} + \frac{\ln(1+Y)}{Y}\right) \qquad (13)$$

A is the element fluoresced

B is the element whose characteristic radiation excites element A radiation

C_B is the concentration of element B

r_A is the absorption edge jump ratio of element A

W(B) is the K or L shell fluorescence yield of element B

A and B are the atomic weights of elements A and B.

U_B is the overvoltage ratio, E_0/E_c, for element B

U_A is the overvoltage ratio, E_0/E_c, for element A

μ_B^A is the mass absorption coefficient of element A for radiation from element B.

μ_B is the mass absorption coefficient of the specimen for radiation from element B.

The absorption parameters X and Y which appear in the above expression are given by:

$$X = (\mu_A/\mu_B) \csc\theta, \quad Y = \sigma/\mu_B \qquad (14)$$

where μ_A is the mass absorption coefficient of the specimen for A radiation, σ is the electron mass absorption coefficient and θ is the take-off angle of the emitted radiation. P_{ij} takes account of the extra factor required in K-L and L-K fluorescence, where j represents the excited line (K_α, K_β, L_α) and i represents the excitation line (K_α, K_β, L_α). When only certain lines of K or L spectrum produce fluorescence excitation special precautions must be taken. The value of $(r_A - 1)/r_A$ for L radiation is equal to 0.75 (Reed).[5]

The correction for fluorescence by the x-ray continuum has been developed by Henoc [15] and by Springer.[16] Generally it has been thought to be a small correction. Recently however, Brown, et al.[17] have shown that this correction is larger than often considered in the past. At this time our computer program does not include this correction.

III. GENERAL DESCRIPTION OF THE PROGRAM

A. Flow Diagram -- The microprobe correction program is designed to run in either of 2 modes. Mode 1 allows one to compute the composition of the sample of interest from measured data (I_A and I (A). Mode 2 allows one to calculate the expected intensity ratios ($I_A/I(A)$) from the known composition of the sample. The flow diagram for the correction program is given in Figure 7.

1. Mode 1 -- The input data contains the parameters necessary for the calculation steps and the raw intensity data from both sample and standards. The raw intensity data is then compiled and the background, dead time and drift corrections are made. The mass absorption coefficients for all the elements analyzed and for all the elements which are present in both samples and standards are then calculated using the method of Heinrich.[6] The corrections, ZAF, (Z is the atomic number correction, A is the absorption correction and F is the fluorescence correction) are then computed for the elements measured in each of the standards in turn (Equations 6, 8 and 12). If any of the standards are pure elements (C(A) = 1.0) no secondary fluorescence correction, F, is made.

The intensity data from the first sample data point is divided by the intensity from the corresponding element standard to obtain the measured intensity ratio, $I_A/I(A)$. This procedure is repeated for all the elements measured in the first sample data point. Then an initial estimate of the composition of all the elements measured in the sample, $C^\circ_{unknown}$, is made by assuming the linear relation

$$C^\circ_{unknown} = C_A = (I_A/I(A))_{measured} C(A). \qquad (15)$$

If there are any elements in the sample which are not measured, their compositions are read into the program as input. If the sample contains oxygen, a corresponding oxygen content is calculated from the assumed cation content of each element in the sample. The total amount of oxygen in the sample is then obtained to be used in the following calculations. The ZAF corrections are applied to the values of $C^\circ_{unknown}$ and a calculated value of I_A is obtained, $(I_A)_{calc}$:

$$(I_A)_{calc.} = (ZAF)\, C^{\circ}_{unknown} \tag{16}$$

The calculated intensity ratio for each element of interest is then obtained, $k_{calc} = (I_A / I(A))_{calc}$. A new estimate of the composition C'_A can then be determined for each element from the equation:

$$C'_{unknown} = \frac{(I_A/I(A))_{measured}}{(I_A/I(A))_{calculated}} \times C^{\circ}_{unknown} \tag{17}$$

A test for the convergence of each element is made in the following fashion:

$$\text{if} \quad \left| \frac{(I_A/I(A))_{calculated}}{(I_A/I(A))_{measured}} - 1 \right| < 5 \times 10^{-3} \tag{18}$$

sufficient convergence has occurred. If any of the elements do not converge, another iteration with new values of $C'_{unknown}$ is made. Iterations are continued until convergence is achieved for all elements.

When convergence is achieved, the calculated compositions are read out. The next point on the sample or another sample is selected and the calculations are repeated. It is only necessary to use new standards and re-calculate standard corrections when a new problem is introduced.

2. Mode 2 – In this mode the compositions of both the standard and sample are input as data. One iteration of the correction procedure is made in order to calculate the intensity ratios, $(I_A/I(A))_{calculated}$ for each element in the sample.

B. Structure of the Computer Program

The program is written in the Fortran IV language according to specifications for its use on IBM S/360 computers. It is built up in modular form using subroutines each of which performs one task. A listing of the program and a glossary of terms used in the conversion program are given in the Appendices I and II respectively. Detailed flow charts and descriptions of the most important subroutines are found in Appendix III. These can be used when the program is modified or initially set up on another type of computer. The subroutines are described briefly in the following paragraphs.

MAIN – Organizes the input data, directs execution of the subroutines, calculates σ (Equation 11), which is used in the absorption and fluorescence corrections, and coordinates the output of the final results.

DATPTS – Associates for each of the measured elements, the standard background and sample intensity values as well as the time for analysis. It also associates the intensity values with the spectrometers used and with the compositions of the standards used for each element. DATPTS inputs the intensities measured by the probe to MAIN after calculating intensity in counts per second and is the one subroutine which is most dependent on the equipment which records the microprobe data (scalers, data translator, typewriter or tape readout). Therefore this is the routine which users will probably wish to tailor to their individual equipment.

MODIFY – Computes the drift correction, if necessary, to be applied to the measured data. It also calculates dead time and background corrections for the measured standards and samples.

ABSCO – Computes the mass absorption coefficients, according to Heinrich,[6] for K_α, K_β and L_α radiation from all the elements present in both the standards and samples as absorbed by each of these elements. Some of these cannot be determined[6] and are calculated as zero.

ATNCOR – Computes the atomic number correction for the standards and samples.

INTERP – Interpolates linearly from the table for R given by Duncumb and Reed[4] to obtain the value of the backscatter coefficient. The coefficient R is a function of both the atomic number of the element of interest, Z, and the reciprocal of the overvoltage, 1/U.

ABSCOR – Computes the absorption correction for any measured element in either sample or standard.

FLUCOR – Computes the secondary fluorescence correction for K or L radiation produced by either K_α, K_β or L_α radiation from any element present in either sample or standard. The total fluorescence correction (Equations 12-14)

$$\left[1 + \sum_i I_f/I_p\right]$$

is obtained by the summation of the effect from the various elements in the sample.

TEST – Determines whether secondary fluorescence by a sample matrix element can excite the element of interest. This is done by determining whether the K_α, K_β and L_α line produced by each element present in the sample is less than the K or L edge of the measured element.

CHANGE – Calculates a new estimate for the composition of the unknown (Equation 17) at the end of each iteration.

ENDIT – Tests for convergence of each element in the sample at the end of each iteration (Equation 18). If convergence is achieved for all elements the composition of the sample is printed out.

OXYGEN – Calculates the amount of oxygen associated with each cation i if oxygen is present in the sample. The following equation is used to calculate the oxygen content:

$$C_{oxy} \text{ for cation } i = \frac{16 C_i}{A_i OX_i} \tag{19}$$

where OX_i = N/M if the oxide has the stoichiometric formula $A_N O_M$.
C_i = wt. % of element i
A_i = atomic weight of element i

The total amount of oxygen present in the sample is given by

$$C_{oxy}\,(total) = 16 \sum_{i=1}^{N} \frac{C_i}{A_i OX_i} + C_o \tag{20}$$

where N is the number of measured cations in the sample and C_o is the amount of oxygen associated with cations in the sample which are not measured. C_o is given as input data.

IV. INPUT TO THE PROGRAM

The input data for the program includes all the necessary physical parameters and compositional information for calculation of the corrections. If Mode 1 is used the measured intensity data are also included as input. The method of input used for the program is a compromise between incorporating many of the parameters into the basic program, which uses up computer storage, and developing very flexible input which increases the time required for the analyst

to organize and run a problem. The input data are broken up into four files which are considered separately.

A. Data File – This file contains the parameters which describe the individual problem and operating conditions of the electron probe.

B. Element File – This file contains the parameters which are a function of a particular element. This file is already available and the elements which will be considered in the problem are selected by the analyst before the run is made.

C. Composition File – This file contains the composition of the standards used for the analysis. The standards are usually available well in advance of a particular run. The data contained in the composition file are often stored on cards or at the computer.

D. Intensity Data File – This file contains the intensity readings from the probe. In many cases, punched tape or cards which are suitable for direct submission to the computer are obtained as output from the microprobe.

The Element file and the Composition file are available beforehand, and in remote terminal usage individual file members can be selected and compiled into the data set for a problem just prior to executed time. The intensity readings from the probe are available or can be made available in suitable form. Therefore, the only input cards that need be punched, before a computer run can be made, are the DATA cards. Sets A, B, C are input in the MAIN program while subroutine DATPTS inputs set D. Appendix IV considers each of the 4 types of input data separately and describes how the input must be set up to make a successful run.

V. OUTPUT FROM THE PROGRAM

We have selected the following output as most important. The element (E) file and selected parameters from the Data File are printed out first. Next the matrix of mass absorption coefficients are given, followed by the raw probe data as it was submitted to the computer.

The correction calculations for the standards are given next: (1) Atomic number correction for each standard, (2) Absorption correction for each element in each standard, (3) Fluorescence correction for each element in each standard. For the first point on each sample, the calculated element compositions are

printed for each iteration step and the ZAF corrections are printed for the final iteration step. For subsequent data points, only the composition values from the first and last iterations are written out.

In Mode 2 problems, the calculated intensity ratios and the ZAF corrections are printed out for each point. In Appendix V the statements which control the output will be discussed as well as methods to change the output statements if desired.

APPENDIX I
Program Listing

MAIN PROGRAM **S.N.**

```
C*************************************************************************      100
C                                                                               200
C                                                                               300
C     MICROPROBE CORRECTION PROGRAM.....MARCH,1969                              400
C                                                                               500
C                                                                               600
C                    J.I.GOLDSTEIN                                              700
C                    DEPARTMENT OF METALLURGY & MATERIALS SCIENCE                800
C                    LEHIGH UNIVERSITY                                          900
C                    BETHLEHEM,PENNSYLVANIA                                    1000
C                                                                              1100
C                    P.A. COMELLA                                              1200
C                    MATHEMATICS AND COMPUTING BRANCH, CODE 642                1300
C                    LABORATORY FOR THEORETICAL STUDIES                        1400
C                                                                              1500
C                    GODDARD SPACE FLIGHT CENTER                               1600
C                    GREENBELT,MARYLAND                                        1700
C                                                                              1800
C                                                                              1900
C                                                                              2000
C*************************************************************************      2100
3      FORMAT('1ELEMENT' 3X,A2,11(8X,A2))                                      2200
4      FORMAT(' ATOM.NO',12F10.4)                                              2300
5      FORMAT(' ATOM.WT',12F10.4)                                              2400
6      FORMAT(' K ALPHA',12F10.4                                               2500
7.     FORMAT(' K BETA ',12F10.4)                                              2600
8      FORMAT(' K EDGE ',12F10.4)                                              2700
9      FORMAT(' L ALPHA',12F10.4)                                              2800
10     FORMAT(' L3 EDGE',12F10.4)                                              2900
11     FORMAT(' CK      ',  12F10.4)                                           3000
12     FORMAT(' NK      ',12F10.4)                                             3100
13     FORMAT(' CKL     ',12F10.4)                                             3200
14     FORMAT(' NKL     ',12F10.4)                                             3300
15      FORMAT(' L1      ',12F10.4)                                            3400
16     FORMAT(' CL1     '12F10.4)                                              3500
17     FORMAT(' L2      ',12F10.4)                                             3600
18     FORMAT(' CL2     ',12F10.4)                                             3700
19     FORMAT(' CLM     ',12F10.4)                                             3800
20     FORMAT(' M1      ',12F10.4)                                             3900
21     FORMAT(' CM1     ',12F10.4)                                             4000
22     FORMAT(' M2      '12F10.4)                                              4100
23     FORMAT(' CM2     ',12F10.4)                                             4200
24     FORMAT(' M3      ',12F10.4)                                             4300
25     FORMAT(' CM3     '12F10.4)                                              4400
26     FORMAT(' M4      '12F10.4)                                              4500
27     FORMAT(' M5      '12F10.4)                                              4600
28     FORMAT(' CMN     '12F10.4)                                              4700
29     FORMAT(' N1      '12F10.4)                                              4800
30     FORMAT(' VC(Z,K)'12F10.4)                                               4900
31     FORMAT(' VC(Z,L)'12F10.4)                                               5000
32     FORMAT(' J1(Z)   '12(I8,2X))                                            5100
33     FORMAT(' RK(Z)   '12F10.4)                                              5200
34     FORMAT(' OXY(Z)  '12F10.4)                                              5300
35     FORMAT(' OMEGA-K'12F10.4)                                               5400
36     FORMAT(' OMEGA-L'12F10.4)                                               5500
37     FORMAT(' LINE    '3X,A2,11(8X,A2))                                      5600
38     FORMAT(' V0      '12F10.4)                                              5700
39     FORMAT(' SPEC.NO',12(I7,3X))                                            5800
40     FORMAT(20A4)                                                            5900
41     FORMAT(I4,10(2X,A2))                                                    6000
```

```
42    FORMAT(4X,10F4.2)                                                      6100
43    FORMAT(' THERE ARE' ,I3,' ELEMENTS IN THIS SAMPLE :' 5X,A2,9(6X,A2     6200
     1 ))                                                                    6300
44    FORMAT('0ATOMIC NUMBER CORRECTION=',F13.5)                             6400
45    FORMAT(                                                                6500
     1    /  '0ABSORPTION CORRECTION FOR ',A2,'.....CHI=',F13.5,7X,          6600
     2 'F(CHI)=',F13.5  )                                                    6700
46    FORMAT(' WEIGHT PERCENTAGES /100 FOR THE ELEMENTS:'F7.4,9F8.4)         6800
47    FORMAT(////,'0',20A4)                                                  6900
48    FORMAT(////'0FINAL CORRECTIONS'//)                                     7000
49    FORMAT(' THETA  ',F10.4 /                                              7100
     1       ' TAU    ' 3E13.5/                                             7200
     2       ' N      ' I7/                                                 7300
     2       ' NM     ' I7/                                                 7400
     2       ' NBGS   ' I7/                                                 7500
     2       ' MODE   ' I7/                                                 7600
     2       ' NPROB  ' I7)                                                 7700
50    FORMAT('1')                                                            7800
51    FORMAT('0ELEMENT  ',A2,'  IS NOT  ACCOUNTED  FOR--NOT  INPUT, NOT      7900
     1 MEASURED, NOT  OXYGEN')                                               8000
67    FORMAT(1X,A2,1X,                                                       8100
     1          I2,2X,F5.1,2(1X,F6.3),1X,I4,1X,F5.2,1X,F6.4,1X,F5.3,3(1X     8200
     1,F6.3),1X,F7.3/4X,F4.2,1X,F6.3,1X,F6.2,1X,F4.2,1X,F6.4,1X,F6.3,5(1     8300
     2X,F6.2)/4X,F5.1,2(1X,F6.3,1X,F4.1),2(1X,F6.3),1X,F5.2,1X,F5.3,1X,      8400
     3F6.5)                                                                  8500
705   FORMAT('0   ATOMIC NUMBER CORRECTION(ANC)  --  ANC=ATN/ATD=(RBU/SB     8600
     1U)*(SBS/RBS)-----(',A2,')-----')                                       8700
706   FORMAT(' ',6X,'ABS =',F10.5/7X,'ABN =',F10.5/7X,'ABD =',F10.5)         8800
707   FORMAT('0   ABSORPTION CORRECTION(ABS)  --  ABS=ABN/ABD-----(',A2,     8900
     1')-----')                                                              9000
710    FORMAT(7X,'ATN='F10.5/7X,'ATD='F10.5/7X,'RBU='F14.5/7X'SBU='F14.5     9100
     1 /7X,'RBS='F14.5/7X'SBS='F14.5////)                                    9200
711   FORMAT(7X,'ANC=',F10.5)                                                9300
713   FORMAT('0   FLUORESCENCE CORRECTION(FLU)  --  FLU=FLN/FLD-----(',A     9400
     12,')-----')                                                            9500
714   FORMAT(' ',6X,'FLU =',F10.5/7X,'FLN =',F10.5/7X,'FLD =',F10.5)         9600
715   FORMAT(////' ELEMENT  CHART   --   WEIGHT  PERCENT'/ 1X,64('-'))       9700
716   FORMAT(' DATA PT     NO ITER ',3X,A2,10(7X,A3))                       9800
717   FORMAT(I5,5X,I5,3X,11(2PF10.3))                                        9900
718   FORMAT(I5,6X,A4,3X,11(2PF10.3))                                       10000
719   FORMAT('0MODE 2 PROBLEM: INPUT-COMPOSITION RATIOS...OUTPUT-INTENSI    10100
     1TY RATIOS'/' PROBLEM#',I5/' ELEMENT.....INTENSITY RATIO-SAMPLE TO     10200
     3STANDARD-ATN*ABN*FLN*C(U)/ATD*ABD*FLD*C(S)'/(4X,A4,10X,F13.5))        10300
720   FORMAT('0IN STANDARD COMBINATION #' I5,2X,A2,' USES STANDARD #'I3)     10400
      DIMENSION OXY(100),STD(9,10),AK(9),                                   10500
     1  AK1(10),UC(10),SC(10),SCON(9,10),ATDS(10),ABDS(9,10),FLDS(9,10),    10600
     1  RBS(10),SBS(10)                                                     10700
      INTEGER*4 STD,U,BSTD                                                  10800
      REAL*4 NK,NKL,L1,L2,L3,M1,M2,M3,M4,M5,N1,KALPHA,KBETA,KEDGE,LALPHA    10900
C                                                                           11000
      NAMELIST /DATA/ THETA,TAU,STD,N,NEU,MODE,V0,LINE,ISPEC,NPROB,         11100
     1  NSTCOM,NM,NBGS,BSTD,M                                               11200
      COMMON/EV/VC(100,2)/JJJ/J1(100)/RVAL/RK(100)/WVAL/OMEGA(100,2)        11300
     A        /F9/ ABCO(50,50,3),SIG,THETA                                 11400
      COMMON /BACK/ BGINT(9,9),BKGR(9),BSTD(9),NBGS ,BTITLE(20,9)           11500
     X        /STAND/ ESTD(10,10),STDINT(9,9,10),NESTD(10),                11600
     Y  CS(10,10),STINTD(9,10,8),COMPST(9,10)                               11700
     X        /SCRIPT/ N,NU(8,3),NM,M ,INDIC                               11800
     X        /INFO/   E(50),Z(50),A(50),KALPHA(50),KBETA(50),KEDGE(50),   11900
     1                 LALPHA(50),L3(50),CK(50),NK(50),CKL(50),NKL(50),    12000
     2                 L1(50),CL1(50),L2(50),CL2(50),CLM(50),M1(50),       12100
     3                 CM1(50),M2(50),CM2(50),M3(50),CM3(50),M4(50),       12200
     4                 M5(50),CMN(50),N1(50)                               12300
     5       /ARGS/ LINE(10),V0,MP,I,LL,LLL,J,NCOUNT                       12400
     X      /CORREC/DRIFT(9,10,8), TAU(3),ISPEC(9)                         12500
     X        /UNKWN/ UINT(75,9,8),NEU,C(10)                               12600
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      X       /XXX/ CHI                                                          12700
      A       /INOUT/ IOUT,IN                                                    12800
       REAL*4 STITLE(20,10),UTITLE(20)                                           12900
       SIGMA(Q,W)= 4.5E5/(Q**1.65-W**1.65)                                       13000
       IOUT=6                                                                    13100
       IN=5                                                                      13200
       DATA LAST,L,O,SUM/'LAST','L',' O','SUM'/                                  13300
100    READ(IN,DATA,END=10000)                                                   13400
       NU(1,1)=1                                                                 13500
        INDIC=1                                                                  13600
       NP1=N+1                                                                   13700
       IS=0                                                                      13800
       DO 125 I=1,M                                                              13900
       READ(IN,67,END=10000) F(I),NO,A(I),VC(I,1),VC(I,2),J1(I),RK(I),           14000
      1   OXY(I),OMEGA(I,1)                                                      14100
      1,KALPHA(I),KBETA(I),LALPHA(I),CK(I),NK(I),KEDGE(I),CKL(I),NKL(I),        14200
      2L1(I),CL1(I),L2(I),CL2(I),L3(I),CLM(I),M1(I),CM1(I),M2(I),CM2(I),        14300
      3  M3(I),CM3(I),M4(I),M5(I),CMN(I),N1(I),OMEGA(I,2)                       14400
       Z(I)=FLOAT(NO)                                                            14500
125    CONTINUE                                                                  14600
       MP=M                                                                      14700
       L=1                                                                       14800
       U=12                                                                      14900
130    IF(M-U) 135,135,160                                                       15000
135    U=M                                                                       15100
160    WRITE(IOUT,3) (F(I),I=L,U)                                                15200
       WRITE(IOUT,4) (Z(I),I=L,U)                                                15300
       WRITE(IOUT,5) (A(I),I=L,U)                                                15400
       WRITE(IOUT,6) (KALPHA(I),I=L,U)                                           15500
       WRITE(IOUT,7) (KBETA(I),I=L,U)                                            15600
       WRITE(IOUT,8) (KEDGE(I),I=L,U)                                            15700
       WRITE(IOUT,9) (LALPHA(I),I=L,U)                                           15800
       WRITE(IOUT,10)(L3(I),I=L,U)                                               15900
       WRITE(IOUT,11)(CK(I),I=L,U)                                               16000
       WRITE(IOUT,12)(NK(I),I=L,U)                                               16100
       WRITE(IOUT,13)(CKL(I),I=L,U)                                              16200
       WRITE(IOUT,14)(NKL(I),I=L,U)                                              16300
       WRITE(IOUT,15)(L1(I), I=L,U)                                              16400
       WRITE(IOUT,16)(CL1(I),I=L,U)                                              16500
       WRITE(IOUT,17)(L2(I),I=L,U)                                               16600
       WRITE(IOUT,18)(CL2(I),I=L,U)                                              16700
       WRITE(IOUT,19)(CLM(I),I=L,U)                                              16800
       WRITE(IOUT,20)(M1(I),I=L,U)                                               16900
       WRITE(IOUT,21)(CM1(I),I=L,U)                                              17000
       WRITE(IOUT,22)(M2(I),I=L,U)                                               17100
       WRITE(IOUT,23)(CM2(I),I=L,U)                                              17200
       WRITE(IOUT,24)(M3(I),I=L,U)                                               17300
       WRITE(IOUT,25)(CM3(I),I=L,U)                                              17400
       WRITE(IOUT,26)(M4(I),I=L,U)                                               17500
       WRITE(IOUT,27)(M5(I),I=L,U)                                               17600
       WRITE(IOUT,28)(CMN(I),I=L,U)                                              17700
       WRITE(IOUT,29)(N1(I),I=L,U)                                               17800
       WRITE(IOUT,30) (VC(I,1),I=L,U)                                            17900
       WRITE(IOUT,31) (VC(I,2),I=L,U)                                            18000
       WRITE(IOUT,32) (J1(I),I=L,U)                                              18100
       WRITE(IOUT,33) (RK(I),I=L,U)                                              18200
       WRITE(IOUT,34) (OXY(I),I=L,U)                                             18300
       WRITE(IOUT,35) (OMEGA(I,1),I=L,U)                                         18400
       WRITE(IOUT,36) (OMEGA(I,2),I=L,U)                                         18500
       WRITE(IOUT,37)(LINE(I),I=L,U)                                             18600
       WRITE(IOUT,39)(ISPEC(I),I=1,N)                                            18700
       IF(U.GE.M) GO TO 175                                                      18800
       L=U+1                                                                     18900
       U=U+12                                                                    19000
       WRITE(6,41) U                                                             19100
       WRITE(6,41) M                                                             19200
       GO TO 130                                                                 19300
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```
175   CONTINUE                                                              19400
      WRITE(IOUT,38) V0                                                     19500
      WRITE(IOUT,49) THETA,(TAU(I),I=1,3),N,NM,NBGS ,MODE                   19600
     1     ,NPROB                                                           19700
      THETA=THETA*3.1415926/180.0                                           19800
      IOX1=0                                                                19900
      DO 200  I=1,NEU                                                       20000
200   IF (E(I).EQ.0) GO TO 300                                              20100
      GO TO 400                                                             20200
300   IOX1=I                                                                20300
400   CONTINUE                                                              20400
      READ(IN,40) (UTITLE(I),I=1,20)                                        20500
      READ(5,2)  (C(I),I=1,NEU)                                             20600
2     FORMAT(8F10.2)                                                        20700
      DO  500  I=1,NEU                                                      20800
500   C(I)= .01*C(I)                                                        20900
      IF(IOX1.GT.0) COXY= C(IOX1)                                           21000
      DO 600 K=1,NM                                                         21100
      READ(IN,40)    (STITLE(I,K),I=1,20)                                   21200
      READ(IN,41)  NEST,(ESTD(I,K),I=1,NEST)                                21300
      READ(IN,2) (CS(I,K),I=1,NEST)                                         21400
      DO 550 I=1,NEST                                                       21500
550   CS(I,K)=.01*CS(I,K)                                                   21600
      NESTD(K)=NEST                                                         21700
600   CONTINUE                                                              21800
      IF(NBGS.EQ.0) GO TO 900                                               21900
      DO 800 K=1,NBGS                                                       22000
      READ(IN,40) (BTITLE(I,K),I=1,20)                                      22100
800   CONTINUE                                                              22200
900   CONTINUE                                                              22300
      IF(NP1.GT.NEU) GO TO 920                                              22400
      DO 910 I=NP1,NEU                                                      22500
      IF(E(I).EQ.0) GO TO 910                                               22600
      IF(C(I).GE.1.E-5) GO TO 910                                           22700
      WRITE(IOUT,51) E(I)                                                   22800
      STOP                                                                  22900
910   CONTINUE                                                              23000
920   DO 930 I=1,M                                                          23100
      IJK=1                                                                 23200
      IF(LINE(I).EQ.L) IJK=2                                                23300
930   LINE(I)=IJK                                                           23400
      CALL ABSCO                                                            23500
      IF(MODE.EQ.1) CALL DATPTS                                             23600
      NCOUNT=1                                                              23700
      DO  4000 K=1,NM                                                       23800
      NEST=NESTD(K)                                                         23900
      CALL ATNCOR(RBS(K),SBS(K),NEST,CS(1,K),ATDS(K),ESTD(1,K))             24000
      WRITE(IOUT,47) (STITLE(I,K),I=1,20)                                   24100
      WRITE(IOUT,43)  NEST,(ESTD(I,K),I=1,NEST  )                           24200
      WRITE(IOUT,46) (CS(I,K),I=1,NEST)                                     24300
      WRITE(IOUT,44) ATDS(K)                                                24400
      DO  3500  I=1,M                                                       24500
      DO  3500  J=1,NEST                                                    24600
      IF (E(I).NE. ESTD(J,K)) GO TO 3500                                    24700
      LLL=Z(I)                                                              24800
      DO  3200 JJ=1,NSTCOM                                                  24900
3200  IF(STD(I,JJ).EQ.K) GO TO 3300                                         25000
      GO TO 3500                                                            25100
3300  LL=LINE(I)                                                            25200
      IF(LLL.GE.37) LL=2                                                    25300
      SIG=SIGMA(V0,VC(I,LL))                                                25400
      SCON(I,K)=CS(J,K)                                                     25500
      CALL ABSCOR(NEST,CS(1,K),ABDS(I,K),ESTD(1,K))                         25600
      WRITE(IOUT,45) E(I),CHI,ABDS(I,K)                                     25700
      FLDS(I,K)=1.                                                          25800
      IF(NEST.GT.1)                                                         25900
     1 CALL FLUCOR(CS(1,K),FLDS(I,K),ESTD(1,K),NEST)                        26000
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```
3500  CONTINUE                                                          26100
4000  CONTINUE                                                          26200
      DO 7000 KKKK=1,NSTCOM                                             26300
      WRITE(IOUT,50)                                                    26400
      DO 7000 IGROUP=1,INDIC                                            26500
      NUP=NU(IGROUP,1)                                                  26600
      DO 7000 NC=1,NUP                                                  26700
      GO TO (4050,4100),MODE                                            26800
4050  NCOUNT=0                                                          26900
      GO TO 4200                                                        27000
4100  NCOUNT=1                                                          27100
4200  DO 5050 I=1,N                                                     27200
      K=STD(I,KKKK)                                                     27300
      SC(I)=SCON(I,K)                                                   27400
      IF(NC.EQ.1)            WRITE(IOUT,720) KKKK,E(I),K                27500
      IF(MODE.EQ.2) GO TO 5050                                          27600
      DR=DRIFT(I,K,IGROUP)*NC                                           27700
      STINT=STINTD(I,K,IGROUP)+DR                                       27800
      AK(I)=UINT(NC,I,IGROUP)/STINT                                     27900
      C(I)=AK(I)*COMPST(I,K)                                            28000
5050  CONTINUE                                                          28100
5075  IF (IOX1.NE.0) CALL OXYGEN(OXY,C,A,  N,IOX1,COXY)                 28200
      SUMM=0.0                                                          28300
      DO 5150 J=1,NEU                                                   28400
      UC(J)=C(J)                                                        28500
5150  SUMM=SUMM+UC(J)                                                   28600
      INDEX=0                                                           28700
      IF(NC.GT.1) GO TO 5200                                            28800
      WRITE(IOUT,715)                                                   28900
      WRITE(IOUT,716) (E(I),I=1,NEU),SUM                                29000
5200  CONTINUE                                                          29100
      WRITE(IOUT,717)NC,INDEX,(UC(I),I=1,NEU),SUMM                      29200
5250  DO 5500 INDEX=1,10                                                29300
472   CONTINUE                                                          29400
       CALL ATNCOR(RBU,SBU,NEU,UC,ATN,E)                                29500
      DO 5400  I=1,N                                                    29600
      K=STD(I,KKKK)                                                     29700
5325  LLL=Z(I)                                                          29800
      LL=LINE(I)                                                        29900
      IF(LLL.GE.37) LL=2                                                30000
      SIG=SIGMA(V0,VC(I,LL))                                            30100
      CALL ABSCOR(NEU,UC,ABN,E)                                         30200
      CALL FLUCOR(UC,FLN,E,NEU)                                         30300
      ANC=ATN/ATDS(K)                                                   30400
      ABS=ABN/ABDS(I,K)                                                 30500
      FLU=FLN/FLDS(I,K)                                                 30600
      AAA=ANC*ABS*FLU                                                   30700
      AK1(I)=AAA*UC(I)/SC(I)                                            30800
      IF(NCOUNT.EQ.0) GO TO 5400                                        30900
      WRITE(IOUT,713) E(I)                                              31000
      WRITE(IOUT,714) FLU,FLN,FLDS(I,K)                                 31100
      WRITE(IOUT,707) E(I)                                              31200
      WRITE(IOUT,706) ABS,ABN,ABDS(I,K)                                 31300
      WRITE(IOUT,705) E(I)                                              31400
      WRITE(IOUT,711)          ANC                                      31500
      WRITE(IOUT,710) ATN,ATDS(K),RBU,SBU,RBS(K),SBS(K)                 31600
5400  CONTINUE                                                          31700
      IF(MODE.EQ.2) GO TO 5550                                          31800
      IF(NCOUNT.EQ.1) GO TO 5575                                        31900
      CALL CHANGE(N,AK1,AK,UC)                                          32000
      IF (IOX1.NE.0) CALL OXYGEN(OXY,UC,A,  N,IOX1,COXY)                32100
      IF(NC.NE.1) GO TO 5475                                            32200
      SUMM=0.                                                           32300
      DO 5450 I=1,NEU                                                   32400
5450  SUMM=SUMM+UC(I)                                                   32500
      WRITE(6,717) NC,INDEX,(UC(I),I=1,NEU),SUMM                        32600
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```
5475  CALL ENDIT(N,AK1,AK,65525)                                          32700
5500  CONTINUE                                                            32800
5525  IF(NC.NE.1) GO TO 5600                                              32900
      NCOUNT=1                                                            33000
      WRITE(IOUT,48)                                                      33100
      GO TO 472                                                           33200
5550  WRITE(6,719) NPROB,(F(I),AK1(I),I=1,N)                              33300
      GO TO 7000                                                          33400
5575  IF(NC.NE.1) GO TO 5600                                              33500
      WRITE(IOUT,715)                                                     33600
      WRITE(IOUT,716) (E(I),I=1,NEU),SUM                                  33700
5600  IF (IOX1.NE.0) CALL OXYGEN(OXY,UC,A,  N,IOX1,COXY)                  33800
      SUMM=0.0                                                            33900
      DO 5625 I=1,NEU                                                     34000
5625  SUMM=SUMM+UC(I)                                                     34100
       INDEX=LAST                                                         34200
5650  WRITE(IOUT,718) NC,INDEX,(UC(I),I=1,NEU),SUMM                       34300
7000  CONTINUE                                                            34400
      GO TO 100                                                           34500
10000 RETURN                                                              34600
      END
```

```
      SUBROUTINE ABSCO                                                    100
      REAL*4 KALPHA,KBETA,KEDGE,LALPHA,LAMBDA                             200
      REAL*4 NK,NKL,L1,L2,L3,M1,M2,M3,M4,M5,N1                            300
      COMMON /SCRIPT/ N,NU(8,3),NM,M                                      400
     X       /INFO/   E(50),Z(50),A(50),KALPHA(50),KBETA(50),KEDGE(50),   500
     1                LALPHA(50),L3(50),CK(50),NK(50),CKL(50),NKL(50),    600
     2                L1(50),CL1(50),L2(50),CL2(50),CLM(50),M1(50),       700
     3                CM1(50),M2(50),CM2(50),M3(50),CM3(50),M4(50),       800
     4                M5(50),CMN(50),N1(50)                              900
     X  /F9/ ABCO(50,50,3)          /INOUT/ IOUT                        1000
      DIMENSION LAMBDA(50)                                               1100
C     THIS SUBROUTINE COMPUTES AND ASSOCIATES THE MASS ABSORPTION COEFFI  1200
      EQ(X1,Y1,Z1)=X1*Y1**Z1                                             1300
      WRITE(IOUT,701)                                                    1400
      DO 801 JUMP=1,3                                                    1500
      GO TO (841,844,842),JUMP                                           1600
  841 DO 851 J=1,M                                                       1700
  851 LAMBDA(J)=KALPHA(J)                                                1800
      GO TO 814                                                          1900
  842 DO 852 J=1,M                                                       2000
  852 LAMBDA(J)=KBETA(J)                                                 2100
      GO TO 814                                                          2200
  844 DO 854 J=1,M                                                       2300
  854 LAMBDA(J)=LALPHA(J)                                                2400
  814 DO 801 I=1,M                                                       2500
      DO 801 J=1,M                                                       2600
      ABCO(I,J,JUMP)=0.0                                                 2700
      IF(LAMBDA(J).EQ.0.) GO TO 801                                      2800
      IF(LAMBDA(J).LT.KEDGE(I)) GO TO 1                                  2900
      IF(L1(I).EQ.0.0)  L1(I)=50.0                                       3000
      IF(LAMBDA(J).LT.L1(I))  GO TO 2                                    3100
      IF (LAMBDA(J).LT.L2(I))  GO TO 3                                   3200
      IF(LAMBDA(J).LT.L3(I))  GO TO 4                                    3300
      IF(LAMBDA(J).LT.M1(I))  GO TO 5                                    3400
      IF(LAMBDA(J).LT.M2(I))  GO TO 6                                    3500
      IF(LAMBDA(J).LT.M3(I))  GO TO 7                                    3600
      IF(LAMBDA(J).LT.M4(I))  GO TO 8                                    3700
      IF(LAMBDA(J).LT.M5(I))  GO TO 9                                    3800
      IF(LAMBDA(J).LE.N1(I))  GO TO 10                                   3900
      GO TO (1000,1100,1000),JUMP                                        4000
 1000 WRITE(IOUT,12) LAMBDA(J),E(J),N1(I),E(I)                           4100
      GO TO 5                                                            4200
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1100  WRITE(IOUT,13) LAMBDA(J),E(J),N1(I),F(I)                          4300
      GO TO 5                                                           4400
    1 ABCO(I,J,JUMP)=CK(I)*LAMBDA(J)**NK(I)                             4500
      GO TO 801                                                         4600
    2 ABCO(I,J,JUMP)=CKL(I)*LAMBDA(J)**NKL(I)                           4700
      GO TO 801                                                         4800
    3 ABCO(I,J,JUMP)=CL1(I)*LAMBDA(J)**NKL(I)                           4900
      GO TO 801                                                         5000
    4 ABCO(I,J,JUMP)=CL2(I)*LAMBDA(J)**NKL(I)                           5100
      GO TO 801                                                         5200
    5 ABCO(I,J,JUMP)=CLM(I)*LAMBDA(J)**2.60                             5300
      GO TO 801                                                         5400
    6 ABCO(I,J,JUMP)=CM1(I)*LAMBDA(J)**2.60                             5500
      GO TO 801                                                         5600
    7 ABCO(I,J,JUMP)=CM2(I)*LAMBDA(J)**2.60                             5700
      GO TO 801                                                         5800
    8 ABCO(I,J,JUMP)=CM3(I)*LAMBDA(J)**2.60                             5900
      GO TO 801                                                         6000
    9 WRITE(6,13) LAMBDA(J)                                             6100
      GO TO 801                                                         6200
   10 ABCO(I,J,JUMP)=CMN(I)*LAMBDA(J)**2.22                             6300
  801 CONTINUE                                                          6400
      WRITE(IOUT,701)                                                   6500
      DO 901 JUMP=1,3                                                   6600
      GO TO (1200,1300,1400),JUMP                                       6700
1200  WRITE(IOUT,702)                                                   6800
       GO TO 1500                                                       6900
1300  WRITE(IOUT, 706)                                                  7000
      GO TO 1500                                                        7100
1400  WRITE(IOUT,705)                                                   7200
1500  L=1                                                               7300
      MI=MINO(14,M)                                                     7400
1550  WRITE(IOUT,703) (F(I),I=L,MI)                                     7500
      DO 1600 I=1,M                                                     7600
1600  WRITE(IOUT,704) F(I),(ABCO(I,J,JUMP),J=L,MI)                      7700
      IF (MI.GE.M) GO TO 901                                            7800
      L=MI+1                                                            7900
      MI=MINO(MI+14,M)                                                  8000
      GO TO 1550                                                        8100
901   CONTINUE                                                          8200
  701 FORMAT('1CORRECTION   VALUES  (FIRST DATA POINT ,  LAST ITERATION  8300
     1)'/1X,57('-'))                                                    8400
  702 FORMAT('    MASS  ABSORPTION  COEFFICIENTS (EMITTER AT TOP)  --  K 8500
     1ALPHA RADIATION')                                                 8600
  703 FORMAT(14(7X,A2))                                                 8700
  704 FORMAT(1X,A2,2X,14(F7.1,2X))                                      8800
  705 FORMAT('    MASS  ABSORPTION  COEFFICIENTS (EMITTER AT TOP)  --  K 8900
     1BETA RADIATION')                                                  9000
  706 FORMAT('    MASS  ABSORPTION  COEFFICIENTS (EMITTER AT TOP)  --  L 9100
     1ALPHA RADIATION')                                                 9200
12    FORMAT(' LAMBDA-K(',F6.3,') OF 'A4,' IS GREATER THAN N1(',F6.3,   9300
     1     ') OF 'A4)                                                   9400
13    FORMAT(' LAMBDA-L(',F6.3,') OF 'A4,' IS GREATER THAN N1(',F6.3,   9500
     1     ') OF 'A4)                                                   9600
      END                                                               9700
```

```
      SUBROUTINE ABSCOR (NEL,C,AB,EL)                                   100
      REAL*4 EL(10),C(10)                                               200
      COMMON/XXX/X                                                      300
     1       /INFO/ E(50),Z(50),A(50)                                   400
     3        /F9/ ABCO(50,50,3),SIG,THETA                              500
     4       /ARGS/ LINE(10),V0,M,I,KK                                  600
      AAVE=0.0                                                          700
      ZAVE=0.0                                                          800
      X=0.0                                                             900
```

```
      DO 2 J=1,NEL                                                          1000
      DO 2 K=1,M                                                            1100
      IF(E(K).NE.EL(J)) GO TO 2                                             1200
      AAVE=AAVE+C(J)*A(K)                                                   1300
      ZAVE=ZAVE+C(J)*Z(K)                                                   1400
      X=X+C(J)*ARGO(K,I,KK)                                                 1500
    2 CONTINUE                                                              1600
      H=1.2*AAVE/ZAVE**2                                                    1700
      X=X/SIN(THETA)                                                        1800
      AB=(1.0+H)/((1.0+X/SIG)*(1.0+H*(1.0+X/SIG)))                          1900
      RETURN                                                                2000
      END                                                                   2100
      .

      SUBROUTINE ATNCOR (RB,SB,NEL,C,AT,EL)                                  100
      DIMENSION EL(10),C(10)                                                 200
      COMMON/EV/VC(100,2)/JJJ/J(100)                                         300
     1       /INFO/ E(50),Z(50),A(50)                                        400
     2       /ARGS/LINE(10),V0,M                                             500
      RB=0.0                                                                 600
      SB=0.0                                                                 700
      DO 1000 I=1,M                                                          800
      DO 500 K=1,NEL                                                         900
500   IF(E(I).EQ.EL(K)) GO TO 600                                           1000
      GO TO 1000                                                            1100
600   L=Z(I)                                                                1200
      LL=LINE(I)                                                            1300
      IF(L.GE.37)  LL=2                                                     1400
      V=.5*(V0+VC(I,LL))                                                    1500
      RECU=VC(I,LL)/V0                                                      1600
      CALL INTERP(RECU,L,RAB)                                               1700
      RB=RB+C(K)*RAB                                                        1800
      S=Z(I)/A(I)*ALOG((1.166E3*V/J(I)))                                    1900
      SB=SB+C(K)*S                                                          2000
1000  CONTINUE                                                              2100
      AT=RB/SB                                                              2200
      RETURN                                                                2300
      END                                                                   2400

      SUBROUTINE CHANGE (N,AK1,AK,UC)                                        100
      DIMENSION AK1(10),AK(10),UC(10)                                        200
C     THIS SUBROUTINE GIVES NEW VALUES FOR THE WEIGHT PERCENTS               300
      DO 200 I=1,N                                                           400
      J=I                                                                    500
100   RAT=AK(I)/AK1(I)                                                       600
      UC(J)=RAT*UC(J)                                                        700
200   CONTINUE                                                               800
      RETURN                                                                 900
      END                                                                   1000

      SUBROUTINE DATPTS                                                      100
      INTEGER*4 BSTD ,SAME                                                   200
      REAL*4 TBG(9,3),TSTD(9,10,3),XINT(3)                                   300
      COMMON/SS/S(3)                                                         400
      COMMON /BACK/ BGINT(9,9),BKGR(9),BSTD(9),NBGS                          500
     X        /SCRIPT/ N,NU(8,3),NM,M,INDIC                                  600
     X       /STAND/ ESTD(10,10),STDINT(9,9,10),NESTD(10)                    700
     X       /UNKWN/ UINT(75,9,8)                                            800
     X      /INOUT/ IOUT,IN                                                  900
     X     /INFO/ E (50)                                                    1000
      WRITE(IOUT,701)                                                       1100
      DO 100 K=1,NM                                                         1200
      DO 50 L=1,9                                                           1300
      DO 40 J=1,3                                                           1400
      TSTD(L,K,J)=0.                                                        1500
```

```
40      CONTINUE                                                                1600
        DO 50 J=1,N                                                             1700
50      STDINT(L,J,K)=0.                                                        1800
100     CONTINUE                                                                1900
        IF(NBGS.EQ.0) GO TO 275                                                 2000
        DO 250 K=1,NBGS                                                         2100
        DO 200 J=1,3                                                            2200
        TBG(K,J)=0.                                                             2300
200     CONTINUE                                                                2400
        DO 250 J=1,N                                                            2500
        BGINT(J,K)=0.                                                           2600
250     CONTINUE                                                                2700
275     CONTINUE                                                                2800
        DO 280 L=1,8                                                            2900
        DO 280 I=1,3                                                            3000
280     NU(L,I)=0                                                               3100
        DO 20000 ICT=1,2000                                                     3200
3000    READ(IN,1)          TIME,XINT,SAME,NUMRDG,INDIC,NOST,IUNK,LAST          3300
        GO TO (3025,3050,3075),NUMRDG                                           3400
3025    IT=1                                                                    3500
        INDMAX=MINO(N,3)                                                        3600
        GO TO (4000,5000,6000),SAME                                             3700
3050    IT=2                                                                    3800
        NUMRDG=4                                                                3900
        INDMAX=MINO(N,6)                                                        4000
        GO TO (4000,5000,6000),SAME                                             4100
3075    IT=3                                                                    4200
        NUMRDG=7                                                                4300
        INDMAX=MINO(N,9)                                                        4400
        GO TO (4000,5000,6000),SAME                                             4500
4000    NU(INDIC,IT)=NU(INDIC,IT)+1                                             4600
        WRITE(IOUT,702)                                                         4700
      1 S(SAME),NU(INDIC,IT),TIME,XINT                                          4800
      2       ,NUMRDG,INDIC   ,(E(J),J=NUMRDG,INDMAX)                           4900
        K=0                                                                     5000
        DO 4100 J=NUMRDG,INDMAX                                                 5100
        K=K+1                                                                   5200
        UINT(NU(INDIC,IT),J,INDIC)=XINT(K)/TIME                                 5300
4100    CONTINUE                                                                5400
        GO TO 20000                                                             5500
5000    TSTD(INDIC,NOST,IT)=TSTD(INDIC,NOST,IT)+TIME                            5600
5050    K=0                                                                     5700
        DO 5100 J=NUMRDG,INDMAX                                                 5800
        K=K+1                                                                   5900
        STDINT(INDIC,J,NOST)=STDINT(INDIC,J,NOST)+XINT(K)                       6000
5100    CONTINUE                                                                6100
        WRITE(IOUT,702)S(SAME),NOST,TIME,XINT,NUMRDG,INDIC,                     6200
      1   (E(J),J=NUMRDG,INDMAX)                                                6300
        GO TO 20000                                                             6400
6000    TBG(NOST,IT)=TBG(NOST,IT)+TIME                                          6500
6050    K=0                                                                     6600
        DO 6100 J=NUMRDG,INDMAX                                                 6700
        K=K+1                                                                   6800
        BGINT(J,NOST)=BGINT(J,NOST)+XINT(K)                                     6900
6100     CONTINUE                                                               7000
        WRITE(IOUT,702)S(SAME),NOST,TIME,XINT,NUMRDG,INDIC,                     7100
      1   (E(J),J=NUMRDG,INDMAX)                                                7200
20000   IF (LAST.NE.0) GO TO 21000                                              7300
21000   DO 21500 K=1,NM                                                         7400
        DO 21400  I=1,INDIC                                                     7500
        DO 21200 J=1,N                                                          7600
        GO TO (21010,21010,21010,21020,21020,21020,21030,21030,21030),J         7700
21010   IT=1                                                                    7800
        GO TO 21040                                                             7900
21020   IT=2                                                                    8000
        GO TO 21040                                                             8100
21030   IT=3                                                                    8200
```

```
21040 IF (TSTD(I,K,IT).NE.0)STDINT(I,J,K)=STDINT(I,J,K)/TSTD(I,K,IT)          8300
21200 CONTINUE                                                               8400
21400 CONTINUE                                                               8500
21500 CONTINUE                                                               8600
      IF(NBGS.EQ.0) GO TO 23000                                              8700
      DO 22000 K=1,NBGS                                                      8800
      DO 21600 J=1,N                                                         8900
      IF(BSTD(J).NE.K) GO TO 21600                                           9000
      GO TO (21510,21510,21510,21520,21520,21520,21530,21530,21530),J        9100
21510 IT=1                                                                   9200
      GO TO 21540                                                            9300
21520 IT=2                                                                   9400
      GO TO 21540                                                            9500
21530 IT=3                                                                   9600
21540 BGINT(J,K)=BGINT(J,K)/TBG(K,IT)                                        9700
21600 CONTINUE                                                               9800
22000 CONTINUE                                                               9900
23000  INDIC=INDIC-1                                                        10000
      GO TO (25000,25000,25000,23100,23100,23100,23300,23300,23300),N       10100
23100  DO 23200 I=1,INDIC                                                   10200
23200  NU(I,1)=MINO(NU(I,1),NU(I,2))                                        10300
      GO TO 25000                                                           10400
23300 DO 24000 I=1,INDIC                                                   10500
24000 NU(I,1)=MINO(NU(I,1),NU(I,2),NU(I,3))                                10600
25000 CALL MODIFY                                                          10700
      RETURN                                                               10800
  701 FORMAT('1INPUT  INFORMATION'/1X,19('-')/'0TYPE  NUMBER  TIME    ',   10900
     13('INTENSITY    '),'NUMRDG',3X,'INDIC',5X,'ELEMENT',5X,'ELEMENT',    11000
     2  5X,'ELEMENT')                                                      11100
702   FORMAT('0',A2,3X,I5,2X,F7.2,3(2X,F11.1),I9,I8,8X,A2,10X,A2,10X,A2)   11200
1     FORMAT(F6.0,3F8.0,1X   ,4I1,I2,I1)                                   11300
    7 FORMAT(' ',A5)                                                       11400
      END                                                                  11500
```

```
      SUBROUTINE ENDIT (N,AK1,AK,*)                                          100
      DIMENSION AK1(10),AK(10)                                               200
C     THIS SUBROUTINE TELLS WHETHER OR NOT TO STOP ITERATING                 300
      ICON=0                                                                 400
      DO 36 I=1,N                                                            500
      IF( ABS(AK1(I)/AK(I)-1.).GT.5.0-3) ICON=ICON+1                         600
   36 CONTINUE                                                               700
      IF(ICON.EQ.0) RETURN 1                                                 800
      RETURN                                                                 900
      END                                                                   1000
```

```
      SUBROUTINE FLUCOR (C,FL,EL,NEL)                                        100
      COMMON/RVAL/OMEGA(100,2)/RVAL/RK(100)/EV/VC(100,2)                     200
      COMMON/XXX/X                                                           300
     1       /INFO/ E(50),Z(50),A(50)                                        400
     5       /INOUT/ IOUT                                                    500
     3        /F9/ ABCQ(50,50,3),SIG,THETA                                   600
     4       /ARGS/ LINE(10),V0,M,L,LL,LLL,I,NCOUNT                          700
      REAL*4 LORK(2) /'K','L'/                                               800
      REAL*8 KAKBLA(6)/2*'K ALPHA ',2*'K BETA  ',2*'L ALPHA '/               900
      DIMENSION EL(10),C(10),ITEST(6),P(6)                                  1000
      DATA P/1.0,0.24,0.1,0.024,4.2,1.0/                                    1100
      UA=V0/VC(L,LL)                                                        1200
      AR=RK(L)                                                              1300
      FL=1.0                                                                1400
      DO 5 J=1,M                                                            1500
      DO 5 IJ=1,NEL                                                         1600
      IF(E(J).NE.EL(IJ)) GO TO 5                                            1700
      CALL TEST(J,L,ITEST)                                                  1800
      SFK=0.0                                                               1900
      DO 4 K=LL,6,2                                                         2000
      IF(ITEST(K).NE.1) GO TO 4                                             2100
      GO TO (125,125,150,150,175,175),K                                     2200
```

```
C       KALPHA RADIATION                                                    2300
125     K1=1                                                                2400
        KK=1                                                                2500
        GO TO 200                                                           2600
C       KBETA RADIOATION                                                    2700
150     K1=3                                                                2800
        KK=1                                                                2900
        GO TO 200                                                           3000
C       LALPHA RADIATION                                                    3100
175     K1=2                                                                3200
        KK=2                                                                3300
200     KAY=Z(J)                                                            3400
        IF(VC(J,KK).EQ.0.) GO TO 4                                          3500
        IF(ABCO(J,J,K1).EQ.0.0)  GO TO 4                                    3600
        UB=V0/VC(J,KK)                                                      3700
        DEN=0.0                                                             3800
        DO 3 K2=1,M                                                         3900
        DO 3 JJ=1,NEL                                                       4000
        IF(F(K2).NE.EL(JJ)) GO TO 3                                         4100
        DEN=DEN+C(JJ)*ABCO(K2,J,K1)                                         4200
      3 CONTINUE                                                            4300
        XF=X/DEN                                                            4400
        Y=SIG/DEN                                                           4500
        IF(LL.EQ.2)AR=4.0                                                   4600
        FK=.5*P(K)*(1.-1./AR)*OMEGA(   J,KK)*(A(L)/A(J))*((UB-1.)/(UA-1.))  4700
       1**1.67*(ABCO(L,J,K1)/DEN)*((ALOG(1.+XF)/XF)+(ALOG(1.+Y)/Y))         4800
        FK=C(IJ)*FK                                                         4900
        SFK=SFK+       FK                                                   5000
        ITEST(K)=0                                                          5100
        IF(NCOUNT.EQ.1) WRITE(IOUT,712) F(J),KAKBLA(K),F(L),LORK(LL),FK,    5200
       1  F(J),C(IJ)                                                       5300
      4 CONTINUE                                                            5400
        FL=FL+SFK                                                           5500
      5 CONTINUE                                                            5600
        IF(NCOUNT.NE.1) RETURN                                              5700
        IF( FL.NE.1) GO TO 400                                              5800
        WRITE(IOUT,713) E(L)                                                5900
        RETURN                                                              6000
400     WRITE(IOUT,714) F(L),FL                                             6100
        RETURN                                                              6200
712     FORMAT(' ',A2,'-',A8,' FLOURESCED ',A2,'-',A2,'.',5X,'KF=',F13.5,   6300
       1   7X,'C( ',A2,' )=',F13.5)                                         6400
713     FORMAT(' NO ELEMENT FLOURESCED ',A2,'...KF(TOTAL)=  1.0',    )      6500
714     FORMAT(' TOTAL FLOURESCENCE CORRECTION FOR ',A2,'=',F13.5)          6600
        END                                                                 6700
```

```
        SUBROUTINE INTERP (RECU,IZ,RAB)                                     100
        COMMON/RA/R(11,11)                                                  200
        DO 1 K=1,10                                                         300
        IF(IZ.LE.K*10) GO TO 3                                              400
      1 CONTINUE                                                            500
      3 I1=K                                                                600
        I2=I1+1                                                             700
        IF(RECU.LE..1) GO TO 7                                              800
        DO 6 L=2,10                                                         900
        AL=L                                                               1000
        IF(RECU.LE.AL*.1) GO TO 8                                          1100
      6 CONTINUE                                                           1200
      7 J1=1                                                               1300
        R=.01                                                              1400
        GO TO 9                                                            1500
      8 J1=L                                                               1600
        R=(AL-1.)*.1                                                       1700
```

```
 9 J2=J1+1                                                                1800
   IF(J1.EQ.1) GO TO 10                                                   1900
   X=.10                                                                  2000
   GO TO 11                                                               2100
10 X=.09                                                                  2200
11 Y=10.0                                                                 2300
   RAB1=R(I1,J1)+((RECU-R)/X)*(R(I1,J2)-R(I1,J1))                         2400
   RAB2=R(I2,J1)+((RECU-R)/X)*(R(I2,J2)-R(I2,J1))                         2500
   RAB=RAB1+((IZ-10*(K-1))/Y)*(RAB2-RAB1)                                 2600
   RETURN                                                                 2700
   END                                                                    2800

   SUBROUTINE MODIFY                                                       100
   INTEGER*4 BSTD                                                          200
   COMMON /BACK/ BGINT(9,9),BKGR(9),BSTD(9),NBGS,BTITLE(20,9)              300
  X       /STAND/ ESTD(10,10),STDINT(9,9,10),NESTD(10),                    400
  X    CS(10,10),STINTD(9,10,8),COMPST(9,10)                               500
  X       /UNKWN/ UINT(75,9,8),NEU,C(10)                                   600
  3         /INFO/ E(25)          /INOUT/ IOUT                             700
  4         /SCRIPT/ N,NU(8,3),NM,M,INDIC                                  800
  5         /CORREC/ DRIFT(9,10,8),TAU(3),ISPEC(9)                         900
   DEADT(X,Y)=X/(1-X*Y)                                                  1000
   DO 4000 I=1,N                                                         1100
   BKGR(I)=0.                                                            1200
       IF (NBGS.EQ.0) GO TO 1000                                         1300
C      BACKGROUND CORRECTIONS                                            1400
       K=BSTD(I)                                                         1500
       IF(K.EQ.0) GO TO 1000                                             1600
       BKGR(I)=BGINT(I,K)                                                1700
       WRITE(IOUT,1) (BTITLE(J,K),J=1,20),BKGR(I)                        1800
1      FORMAT(' ',20A4,5X,E13.5,' COUNTS/SECOND'                         1900
1000   JJ=ISPEC(I)                                                       2000
       DO 2000 K=1,NM                                                    2100
       NEST=NESTD(K)                                                     2200
       DO 1100  J=1,NEST                                                 2300
       IF(E(I).EQ.ESTD(J,K)) GO TO 1150                                  2400
1100   CONTINUE                                                          2500
       GO TO 2000                                                        2600
C      DRIFT CORRECTIONS                                                 2700
1150    DO 1600 L=1,INDIC                                                2800
       DRIFT(I,K,L)=0.                                                   2900
       L1=L+1                                                            3000
       IF(ABS(STDINT(L1,I,K)-STDINT(L,I,K)).GE.6.*SQRT(STDINT(L,I,K)))   3100
      1DRIFT(I,K,L)=(STDINT(L1,I,K)-STDINT(L,I,K))/NU(L,1)               3200
C      STANDARD INTENSITY CORRECTIONS                                    3300
1500   CONTINUE                                                          3400
       STINTD(I,K,L)=DEADT(STDINT(L,I,K),TAU(JJ))-BKGR(I)                3500
1600   CONTINUE                                                          3600
       COMPST(I,K)=CS(J,K)                                               3700
2      FORMAT(3I4,9E13.5)                                                3800
2000   CONTINUE                                                          3900
C      DEAD TIME AND BACKGROUND CORRECTIONS TO UNKNOWN                   4000
       DO 3500 L=1,INDIC                                                 4100
       NUP=NU(L,1)                                                       4200
       DO 3000 J=1,NUP                                                   4300
3000   UINT(J,I,L)=DEADT(UINT(J,I,L),TAU(JJ))-BKGR(I)                    4400
3500   CONTINUE                                                          4500
4000   CONTINUE                                                          4600
       RETURN                                                            4700
       END                                                               4800
```

```
      SUBROUTINE OXYGEN (OX,C,A,N,IOX,COX)                              100
      DIMENSION OX(100),C(10),A(10),Z(10)                               200
      CT=0.                                                             300
      DO 100 I=1,N                                                      400
100   CT=CT+C(I)/(OX(I)*A(I))                                           500
      C(IOX)=COX+16.*CT                                                 600
      RETURN                                                            700
      END                                                               800

      SUBROUTINE TEST (KKK,LLL,ITEST)                                   100
      REAL*4 KALPHA,KBETA,KEDGE,LALPHA,LEDGE                            200
      COMMON /INFO/ SPACE(150),KALPHA(50),KBETA(50),KEDGE(50),          300
     1  LALPHA(50),LEDGE(50)                                            400
      DIMENSION ITEST(6)                                                500
      DO 100 I=1,6                                                      600
100   ITEST(I)=0                                                        700
      IF(KALPHA(KKK).LT.KEDGE(LLL)) ITEST(1)=1                          800
      IF(KALPHA(KKK).LT.LEDGE(LLL)) ITEST(2)=1                          900
      IF(KBETA (KKK).LT.KEDGE(LLL)) ITEST(3)=1                         1000
      IF(KBETA (KKK).LT.LEDGE(LLL)) ITEST(4)=1                         1100
      IF(LALPHA(KKK).LT.KEDGE(LLL)) ITEST(5)=1                         1200
      IF(LALPHA(KKK).LT.LEDGE(LLL)) ITEST(6)=1                         1300
      RETURN                                                           1400
      END                                                              1500
```

```
      BLOCK DATA                                                        100
      COMMON /RA/R(11,11)                                               200
      COMMON/SS/S(3)                                                    300
      DATA R/1.00,.934,.856,.786,.735,.693,.662,.635,.611,.592,.578,    400
     A1.00,.944,.873,.808,.760,.718,.688,.663,.630,.613,.606,1.00,.953, 500
     B.888,.828,.782,.741,.713,.687,.665,.639,.634,1.00,.961,.903,.847, 600
     C.804,.764,.737,.713,.691,.665,.661,1.00,.968,.917,.867,.827,.789, 700
     D.764,.740,.718,.695,.691,1.00,.975,.933,.888,.851,.817,.793,.770, 800
     E.750,.730,.725,1.00,.981,.948,.911,.878,.847,.825,.805,.785,.767, 900
     F.763,1.00,.988,.963,.935,.907,.881,.862,.844,.826,.811,.806,1.00, 1000
     G.993,.977,.959,.938,.919,.904,.889,.874,.862,.858,1.00,.997,.990, 1100
     H.981,.970,.959,.950,.941,.932,.924,.921,11*1.00/                  1200
      DATA S/'U','S','B'/                                               1300
      END                                                               1400
```

APPENDIX II
Glossary of Terms Used in the Microprobe Correction Program

A(I), $1 \leq I \leq M$	Atomic weight of the element, E(I).
AK(I), $1 \leq I \leq N \leq M$	Ratio of the measured intensity readings for E(I) in the unknown to the average corrected intensity reading of E(I) in standard K. (Equation 2).
AK1 (I), $1 \leq I \leq M$	Value of k_A (calculated) at the ith iteration; AK1(I) = AAA* UC(I)/SC(I).
AAA	Product of ZAF. This is calculated separately for each element E(I).
AB	Dummy argument for absorption correction in subroutine ABSCOR.
ABN	Absorption correction for the unknown. This is computed for each element E(I).
ABDS(I, K), $1 \leq I \leq N$, $1 \leq K \leq NM$	Absorption correction for E(I) in standard K.
ABS	Combined absorption correction ABS = ABN/ABDS(I, K).
AT	Dummy argument for the atomic number correction in subroutine ATNCOR.
ATN	Atomic number correction for the unknown.
ATDS(K), $1 \leq K \leq NM$	Atomic number correction for standard K.
ANC	Combined atomic number correction ANC = ATN/ATDS(K)
ABCØ(I, J, K) $1 \leq I \leq M$, $1 \leq J \leq N$, $1 \leq K \leq 3$	Matrix of mass absorption coefficients with E(I) the absorber, E(J) the emitter, at the K_α -line (K = 1), K_β -line (K = 2) or L_α -line (K = 3).

BSTD(I), $1 \leq I \leq N$		If BSTD(I) = K, $1 \leq K \leq 9$, then background standard K is used for E(I). If BSTD (I) = 0, no background correction is necessary.
BKGR(I), $1 \leq I \leq N$		Average background intensity for E(I).
BGINT(I, K)	$1 \leq I \leq N$ $1 \leq K \leq NBGS$	Average background intensity readings for each element E(I) using background standard K in units of counts per second.
BTITLE(J, K), J=1,2 ...20	$1 \leq K \leq NBGS$	Identification card for background standard K.
C(I), $1 \leq I \leq NEU$		Composition (wt%) of E(I) present in the unknown. C is used as a dummy argument denoting the composition of a sample in subroutines FLUCOR, ATNCOR, ABSCOR, OXYGEN
CK(I) CKL(I) CL1(I) CL2(I) CLM(I) CM1(I) CM2(I) CM3(I) CMN(I)	$1 \leq I \leq M$	Constants for computing mass absorption coefficients in subroutine ABCØ where $\mu/\rho = C\lambda^n$.
CS(I,K),	$1 \leq I \leq NESTD(K)$ $1 \leq K \leq NM$	Composition (wt%) of each element (ESTD(I,K)) present in standard K.
CØXY		Wt% oxygen present in the unknown which is given as input, CØX is dummy argument for CØXY in subroutine OXYGEN.
CØMPST(I, K),	$1 \leq I \leq N$ $1 \leq K \leq NM$	Wt% of E(I) present in standard K.
CHI		χ - used in computing absorption correction (Equation 8, 9).
DRIFT(I,K,L),	$1 \leq I \leq N$ $1 \leq K \leq NM$ $1 \leq L \leq INDIC-1$	Total Drift correction to intensity readings for E(I) in standard K. L refers to INDIC-1, the number of times the standards have been measured.

EL	Dummy argument used to specify chemical symbol of each element in a sample. EL is used in subroutines ABSCOR, FLUCOR and ATNCOR.
DR	Drift correction for unknown calculated for each element E(I).
DATA	NAMELIST name which inputs the following parameters: THETA, TAU, STD, N, NEU, MØDE, V0, LINE, ISPEC, NPRØB, NSTCØM, NM, NBGS, BSTD.
E(I)	Array of chemical symbols of all elements used in the problem; this table is ordered as described in Appendix IV (E File).
ESTD(I,K) $1 \leq I \leq NESTD(K)$ $1 \leq K \leq NM$	Array of chemical symbols for the elements E(I) present in the standard K.
FL	Dummy argument for fluorescence correction in subroutine FLUCOR.
FLN	Fluorescence correction for the unknown. If necessary, this is computed for each element E(I) in the unknown.
FLDS(I,K), $1 \leq I \leq N$ $1 \leq K \leq NM$	Fluorescence correction (if any) for E(I) in standard K.
FLU	Combined fluorescence correction FLU = FLN/FLDS(I,K) FLU = 1.0, if no correction.
IN	Specifies which computer input unit is used.
IØUT	Specifies which computer output unit is used.
IØXI	Subscript used to denote whether oxygen is present in the problem. If IØ X 1 = 0, no oxygen If IØ X1 > 0, oxygen is present

ISPEC(I), I = 1,N	Denotes whoch spectrometer was used to measure E(I).
INDIC	The number of times the standards as a group were measured (see Appendix IV, Data set D).
J1(I), I = 1,M	Mean Ionization Potential - Input to MAIN.
J	Mean Ionization Potential - as used in subroutine ATNCOR.
KEDGE (I), I = 1,M	K-edge for E(I)
KALPHA(I), I = 1,M	Wavelength of K_{α}-line for E(I).
KBETA(I), I = 1,M	Wavelength of K_{β}-line for E(I).
LALPHA(I),I = 1,M	Wavelength of L_{α}-line for E(I).
M	The number of different elements used in any problem, $1 \leq M \leq 50$. This includes elements in standards, and unknowns.
N	Number of elements in the unknown measured by the probe.
L1(I), I = 1,M L2(I), I = 1,M L3(I), I = 1,M	Wavelengths associated with the 3 L-edges, L_I, L_{II}, L_{III}; used in subroutine ABCØ to obtain mass absorption coefficients.
M1(I), M2(I), M3(I), M4(I), M5(I), I = 1,M	Wavelengths associated with the 5 M-edges, used in subroutine ABCØ to obtain mass absorption coefficients.
NK(I), I = 1,M	Exponent of λ for each element (I) in the expression for mass absorption coefficient ($\mu/\rho = C\,\lambda^n$) in the wavelength region from 0.7Å to the K-edge of element I.
NKL(I), I = 1,M	Exponent of λ for each element (I) in the expression for mass absorption coefficient ($\mu/\rho = C\lambda^n$) in the wavelength region from the K-edge to the L_{III}-edge of element I.

NI(I), I = 1, M	Wavelength associated with the first N-edge; used in subroutine ABCØ to obtain mass absorption coefficients.
NEU	Total number of elements in the unknown.
NM	Number of standards used in a problem.
NU	Number of readings taken on an unknown sample. NU is obtained by the computer internally.
NC	The number of the unknown sample being analyzed. NC is obtained by the computer internally; $1 \leq NC \leq NU$.
NBGS	Specifies the number of background standards used in the analysis.
NESTD(K) K = 1, NM	Number of elements in standard K
NEST	NEST = NESTD(K)
NSTCØM	See Explanation of input data set A (Appendix IV).
ØXY(I), I = 1,M	ØXY(I) = N/M if the oxide is of the form $E(I)_N O_M$.
ØMEGA(I,K), I = I, M K = 1, 2	Fluorescence yield Ω (I, 1) for K radiation. Fluorescene yield Ω (I, 2) for L radiation.
RB	Dummy argument for backscatter coefficient in ATNCOR.
RBS(K), 1≤ K≤ NM	Backscatter coefficient for standard K.
RBU	Backscatter coefficient for unknown.
RK(I), 1 ≤ I ≤ M	Absorption jump ratio, r, for K lines in each element E(I).
R(I, J), I = 1, 11 J = 1, 11	Tabulated values of R. I indicates the atomic number and J indicates the reciprocal of U = VC/VO.

RECU	Reciprocal of U = VC/VO.
STDINT (J, I, K), J = 1, INDIC 1 ≤ I ≤ N 1 ≤ K ≤ NM	Intensity of each element E(I) in standard K measured in counts per second. J gives the number of times the standards as a whole have been measured.
STINTD(I, K, L), 1≤ I≤ N 1≤ K≤ NM 1≤ L≤ INDIC-1	Intensity readings in counts per second for each element E(I) in standard K after correction for dead time and background.
STITLE(K, J) 1 ≤ K ≤ NM J = 1, 20	Identification card for standard K. See Appendix IV, Input file C.
SIGMA	σ (Equation 11).
SB	Dummy argument for stopping power in ATNCOR.
SBS(K), 1≤ K ≤ NM	Calculated stopping power for each standard K.
SBU	Calculated stopping power for each unknown.
STD(I, J) 1≤ I≤ M 1≤ J≤ NSTCØM	See Appendix IV, input data set A.
STINT	The fully corrected intensity for each element in a standard.
SCON(I, K) 1 ≤ I ≤ M 1≤ K≤ NM	Weight % of element E(I) present in standard K.
TAU(J), J = 1,3	Dead time for spectrometers 1, 2, and 3 respectively.
TBG(K, I), K = 1, NBGS 1≤ I≤ 3	Counting time on background standard K. I indicates which group of elements is being measured.

TSTD(I, K, J) I = 1, INDIC K = 1, NM J = 1, 3	Counting time on standard K. I gives the number of times all of the standards have been measured. J indicates which group of elements is being measured.
THETA	Take off angle of the electron probe.
UINT(NC, J, L) $1 \leq NC \leq NU(L)$ $1 \leq J \leq N$ $1 \leq L \leq INDIC-1$	Intensity reading for an element E(J) in counts per second in the unknown. NC indicates the number of the sample and L indicates the number of times the standards as a whole have been measured.
UTITLE (J), J = 1, 20	Identification card for the unknown.
UC(J), $1 \leq J \leq N$	Calculated wt. % of element E(J) present in the unknown.
VO	Operating voltage.
VC(I, LL) $1 \leq I \leq M$ LL = 1, 2	Excitation energy of each element E(I) for either the K-line (LL = 1) or the L-line (LL = 2).
X	Dummy variable for CHI in subroutine FLUCOR and ABSCOR
Z(I), $1 \leq I \leq M$	Atomic number of E(I).

APPENDIX III
Detailed Descriptions of Subroutines

A. MAIN – This subroutine inputs the data files (A,B,C) and calls DATPTS to input data set (D). For those elements whose compositions are specified in the unknown, it is assumed that these compositions will not vary from unknown sample to unknown sample. MAIN calls for the calculation of mass absorption coefficients, and for each standard calls for the computation of atomic number, absorption and fluorescence corrections. To each element in the unknown MAIN assigns a standard and then calculates in turn an estimate for the composition of the unknown, the corrections associated with the estimated composition and then re-estimates the composition. This is done for each set of intensity readings on the unknown. If MODE = 2, the composition of the sample is known, and the intensity ratios of unknown to standard are calculated for each element. Finally, the MAIN routine outputs a detailed account of the computations to assist the experimenter in his analysis. Figure 1 presents a flow chart of MAIN.

B. DATPTS – DATPTS, as developed for the GSFC microprobe, reads and processes data in the following fashion: Each card, which DATPTS inputs, contains a time and 3 intensity counts, one for each spectrometer, as well as other information outlined for the Intensity Data File (Appendix IV).

If the readings are taken on the sample, the intensities are divided by the time to obtain the number counts per second for each measured element. The total number of data points taken on the sample are then computed. If the readings are taken on the standards or backgrounds, the average intensities and average counts per second are obtained.

When all the readings for the problem have been input, DATPTS calls subroutine MODIFY which computes corrections to the raw data. The flow chart of DATPTS is shown in Figure 2.

C. MODIFY – To each measured element MODIFY assigns a background correction according to the values of NBGS and the BSTD array (Appendix IV). It computes the drift correction for each element standard, storing the corrections in the DRIFT matrix. The count rates for each standard are corrected for dead-time and background and stored in the STINTD matrix. Then the unknown sample count rates are corrected for dead-time and background and restored in the UINT matrix. Figure 3 illustrates the flow of MODIFY.

D. ATNCOR – for each sample this subroutine computes the atomic number correction according to Equations 6-7. The (dummy) arguments of the subroutine are:

RB – the backscatter coefficient
SB – the stopping power
NEL – the number of elements in the sample
AT – the atomic number correction
EL – the element array for the sample.

Figure 4 gives a flow chart of ATNCOR.

E. ABSCOR – computes the absorption correction for each element in each sample (Equations 8-11). NEL, C, EL, AB are the arguments of the subroutine, ABSCOR. The first 3 have the same meaning as in ATNCOR and AB is the absorption correction for the element E(I). The MAIN program selects E(I) and transmits the parameter, I, in the ARGS COMMON block. Figure 5 illustrates the flow of ABSCOR.

F. FLUCOR – computes the fluorescence correction (if any) for each element E(L) in each sample (Equations 12-14). The arguments EL, NEL, C are the same as in ATNCOR; FL is the fluorescence correction and L is transmitted in the ARGS COMMON block. Figure 6 is a flow chart of FLUCOR.

G. TEST – is a subroutine called by FLUCOR to determine if an element, E(J), in a sample has fluoresced the element, E(L), measured for that sample. Whenever fluorescence occurs, the ITEST argument is set to 1; otherwise it remains 0:

If K_α E(J) < K_{edge} E(L), ITEST (1) = 1
K_α E(J) < L_{edge} E(L), ITEST (2) = 1
K_α E(J) < K_{edge} E(L), ITEST (3) = 1
K_β E(J) < K_{edge} E(L), ITEST (4) = 1
L_α E(J) < K_{edge} E(L), ITEST (5) = 1
L_α E(J) < L_{edge} E(L), ITEST (6) = 1

J and L are also transmitted as arguments.

H. INTERP – linearly interpolates from the tabulated values for R given by Duncumb and Reed.[4] This subroutine is used by ATNCOR to compute the value of the backscatter coefficient. The arguments are IZ, the atomic number of E(I); RECU, (1/U); and RAB, the value of R. The values of R^4 are contained in the block data at the end of MAIN.

I. ENDIT – Tests for convergence for each measured element, E(I) in the unknown sample. If sufficient convergence is achieved, Equation 18, then ENDIT directs MAIN to end the iterative procedure and output the final composition of the unknown. If not, ENDIT returns to the iterative portion of MAIN.

APPENDIX IV
Description of Input Files

A-DATA FILE – The Fortran IV namelist feature directs the input of DATA File. This option enables data to be identified by name; for example, I = 1 will cause a 1 to be placed in the location labeled I; E(3) = 'Fe' causes the third item in the E-array to be identified as iron. The parameters initialized in this fashion are described below. The statement in the MAIN program

```
100 READ(IN,DATA,END = 10000)
```

accomplishes the initialization. Figure 8 shows an example of the sample NAMELIST cards for one of the problems presented in Appendix VI.

M is the total number of elements present in both the unknown and standards
NEU is the total number of elements in the unknown
N is the number of elements measured by the probe
NM is the number of standards used in an analysis
NSTCOM is the number of ways in which the standards were combined to determine the composition or intensity ratios for the unknown. This allows different standards to be used for calculation of the same element. For example, if element A appears in both standard #1 and standard #2, the experimenter may wish to use standard #1 first for A to obtain the amount of A present and then standard #2 for the same purpose. Up to 10 such combinations may be made for a problem.

STD(I,J), I = 1, N; J = 1, NSTCOM specifies which standard is to be used for E(I) in standard combination J; for example if STD (4,2) = 3, use standard #3 for E(4) in the second analysis of the data. The standard is designated by number which corresponds to its order in the Composition File.

NBGS specifies the number of background standards used in the analysis: $0 \leq NBGS \leq 9$. This program assumes one background standard per element.

BSTD(I), I = 1, N - If NBGS > 0 there is at least 1 element measured for which the background is non-zero; hence, the BSTD array must be initialized for I = 1, 2, . . ., N, in the following manner. If the background for E(I) is zero, set BSTD(I) = 0; if the background is not 0, set BSTD(I) = K where K is the number of the background standard used for E(I).

MODE – If MODE = 1, intensity readings from the probe (Intensity Data File) are input and the weight % present in the unknown is determined for the measured elements. If MODE = 2 the composition of the unknown is known and the output consists of the intensity ratios of unknown intensity to standard intensity for each element in the unknown.

LINE(I), I = 1, M specifies whether the element, E(I), was measured with the K or L x-ray line.

ISPEC(I), I = 1, N specifies on which spectrometer (first, second, or third, etc.) the element, E(I), was measured.

VO gives the operating voltage for the probe (E_0) in kilovolts.

TAU(I), I = 1, 2, 3 specifies the dead-times for spectrometers, 1,2,3 respectively.

Note: If the probe has more than 3 spectrometers, the dimension on TAU should be increased accordingly.

THETA is the take-off angle given in degrees.

B-Element File

For elements 3-92, file cards are provided for each element. Each of these sets of 3 cards contains the element's chemical symbol, atomic number (Z), atomic weight (A), excitation energies for the K (elements Z = 5-39) and L (elements Z = 12-92) lines in kilovolts (Bearden),[18] mean ionization potential (J_i) in electron volts (Duncumb and Reed),[4] the K absorption jump ratio (r_A) (Colby),[19] the cation to anion ratio if oxide is formed (OX), the K shell fluorescence yield (W(B)) and the mean L shell fluorescence yield (W(B)) (Fink, et al.).[20] the K_α and K_β wavelengths for elements Z = 3-39 and the L_α wavelengths for elements Z = 20-92. For elements less than atomic number 20, the L_α wavelength is set to 50Å. Also given in the E file are the K, L_I, L_{II}, L_{III}, M_I, M_{II}, M_{III}, M_{IV}, M_V, N_I wavelength edges (Bearden)[18] in Å units and the CK, NK, CKL, NKL, CL1, CL2, CLM, CM1, CM2, CM3, CMN parameters used by Henrich[6] to calculate the mass absorption coefficients.

To enable the user to calculate approximate mass absorption coefficients for L lines of elements of atomic number 24-29, values of CL1 and CL2 were determined by linear extrapolation from the values given by Heinrich[6] for elements Z = 30 and above. The complete Element File compiled to date is given in the following Table.

TABLE I
Element File

```
FL  NO. WGT.- VC(K)- VC(L)- -J-- -RK-- -OXY-- OMGAK KALPHA KBETA- LALPHA --CK---
    -NK- KEDGE- --CKL- NKL- --L1-- -CL1-- --L2-- -CL2-- --L3-- -CLM-- --M1--
    -CM1- -M2--- CM2- --M3-- CM3- --M4-- --M5-- CMN-- --N1-- OMGAL
'LI' 3. 007.0 0.0548 00.000 0000 00.00 1.0000 .0000 00.000 00.000 50.000 000.135
    2.88 226.5
                                                                        .00375
'BE' 4. 009.0 00.111 00.000 0000 00.00 1.0000 .0000 00.000 00.000 50.000 000.350
    2.86 111.00
                                                                        .00500
' B' 5. 010.8 00.000 00.000 0000 15.73 0.6667 .0000 67.600 00.000 50.000 000.740
    2.85
                                                                        .00625
' C' 6. 012.0 00.284 00.000 0146 15.14 1.0000 .0009 44.700 00.000 50.000 001.350
    2.84 43.680
                                                                        .00750
' N' 7. 014.0 00.400 00.000 0135 14.59 1.0000 0.002 31.600 00.000 50.000 002.210
    2.83 30.990
                                                                        .00875
' O' 8. 016.0 00.532 00.000 0127 14.08 1.0000 0.004 23.700 00.000 50.000 003.800
    2.82 23.320
                                                                        .01000
' F' 9. 019.0 00.692 00.000 0123 13.60 1.0000 0.007 18.300 00.000 50.000 004.900
    2.81
                                                                        .01125
'NE'10. 020.2 00.867 00.000 0123 13.16 1.0000 0.015 14.600 14.500 50.000 006.770
    2.80 14.300
                                                                        .01250
'NA'11. 023.0 01.070 00.000 0126 12.74 2.0000 0.020 11.910 11.617 50.000 009.050
    2.79 11.480 0.62   2.73
                                                                        .01375
'MG'12. 024.3 01.300 00.049 0133 12.35 1.0000 0.030 09.889 09.558 50.000 011.750
    2.79 09.512 000.89 2.73                                          250.7
                                                                        .01500
'AL'13. 027.0 01.560 00.075 0142 11.99 0.6667 0.042 08.337 07.981 50.000 014.870
    2.78 07.951 001.18 2.73                                          170.4
                                                                        .01625
'SI'14. 028.1 01.840 00.100 0154 11.64 0.5000 0.056 07.126 06.768 50.000 018.500
    2.77 06.738 001.54 2.73                                          123.0
                                                                        .01750
' P'15. 031.0 02.140 00.132 0166 11.31 0.4000 0.075 06.155 05.804 50.000 022.500
    2.76 05.784 002.43 2.73                                           94.0
                                                                        .01875
' S'16. 032.1 02.470 00.000 0180 11.00 1.0000 0.096 05.373 05.032 50.000 027.000
    2.76 05.018 002.43 2.73
                                                                        .02000
'CL'17. 035.5 02.820 00.000 0194 10.71 1.0000 0.117 04.728 04.403 50.000 031.700
    2.76 04.377 002.98 2.73
                                                                        .02125
'AR'18. 039.9 03.200 00.000 0209 10.43 1.0000 0.138 04.193 03.886 50.000 036.900
    2.75 03.871 003.62 2.73
                                                                        .02250
' K'19. 039.1 03.610 00.295 0224 10.17 2.0000 0.159 03.742 03.454 50.000 042.500
    2.75 03.437 004.31 2.73                                           42.1
                                                                        .02375
'CA'20. 040.1 04.040 00.349 0239 09.92 1.0000 0.180 03.359 03.090 36.330 048.400
    2.74 03.070 005.10 2.73                                           35.5
                                                                        .02500
'SC'21. 045.1 04.490 00.000 0255 09.68 1.0000 0.202 03.032 02.780 31.350 055.100
    2.74 02.7620005.99 2.73
                                                                        .02625
```

TABLE I–(continued)

```
EL  NO. WGT.- VC(K)- VC(L)- -J-- -RK-- -OXY-- OMGAK KALPHA KBETA- LALPHA --CK---
    -NK- KFDGF- --CKL- NKL- --L1-- -CL1-- --L2-- -CL2-- --L3-- -CLM-- --M1--
    -CM1- -M2--- CM2- --M3-- CM3- --M4-- --M5-- CMN--- --N1-- OMGAL

'TI'22. 047.9 04.970 00.450 0270 09.45 1.0000 0.224 02.748 02.514 27.420 062.100
    2.73 02.497 007.00 2.73                                    27.3
                                                                        .02750
' V'23. 051.0 05.470 00.000 0286 09.24 1.0000 0.246 02.504 02.284 24.250 069.800
    2.73 02.269 008.02 2.73
                                                                        .02875
'CR'24. 052.0 05.990 00.598 0301 09.03 1.0000 0.268 02.291 02.085 21.640 078.000
    2.73 02.070 009.18 2.73 16.7   7.80   17.9   4.8    20.7
                                                                        .03000
'MN'25. 054.9 06.540 00.000 0316 08.83 1.0000 0.290 02.103 01.910 19.500 086.700
    2.72 01.896 010.45 2.73        8.85           5.9    19.1
                                                                        .03125
'FE'26. 055.9 07.110 00.707 0332 08.64 1.0000 0.320 01.937 01.757 17.600 095.800
    2.72 01.743 011.75 2.73 17.2 ' 10.0   17.2   7.0    17.525
                                                                        .03250
'CO'27. 058.9 07.710 00.779 0347 08.46 1.0000 0.350 01.790 01.621 16.000 105.500
    2.71 01.608 013.25 2.73 15.61  11.25  15.61  8.0    15.92
                                                                        .03375
'NI'28. 058.9 08.330 00.854 0362 08.29 1.0000 0.380 01.659 01.500 14.600 115.900
    2.71 01.488 014.80 2.73 14.2   12.6   14.2   9.0    14.52
                                                                        .03500
'CU'29. 063.5 08.980 00.933 0377 08.12 1.0000 0.410 01.542 01.392 13.400 126.800
    2.71 01.380 016.45 2.73 11.270 014.06 13.01  10.1   13.29
                                                                        .03625
'ZN'30. 065.4 09.660 01.020 0392 07.96 1.0000 0.440 01.436 01.295 12.300 138.000
    2.70 01.283 018.25 2.73 10.330015.60  11.870011.20  12.13
                                                                        .03750
'GA'31. 069.7 10.400 01.120 0407 07.81 1.0000 0.480 01.341 01.208 11.313 149.800
    2.70 01.196 020.20 2.7309.520 017.25  10.830 12.40  11.100
                                                                        .03875
'GE'32. 072.6 11.100 01.220 0422 07.66 1.0000 0.520 01.255 01.128 10.456 162.200
    2.70 01.117 022.15 2.73 08.730 018.95 09.940 013.60 10.190
                                                                        .04000
'AS'33. 074.9 11.900 01.320 0437 07.51 1.0000 0.560 01.177 01.056 09.671 175.400
    2.69 01.045 024.25 2.73 08.107 20.750 09.124 014.90 09.390 004.28
                                                                        .04125
'SE'34. 079.0 12.600 01.430 0451 07.38 1.0000 0.600 01.106 00.990 08.990 189.400
    2.69 00.980 026.40 2.73 07.506 22.550 08.416 16.200 08.670 004.69
                                                                        .04250
'BR'35. 079.9 13.500 01.550 0466 07.24 1.0000 0.640 01.041 00.931 08.375 205.000
    2.69 00.920 028.80 2.73 06.970 24.600 007.80 17.700 008.00 005.13
                                                                        .04375
'KR'36. 083.7 14.300 01.680 0481 07.12 1.0000 0.666 00.981 00.876 00.000 219.300
    2.68 00.866 031.25 2.73 6.4600 26.700 007.21 019.15 007.43 005.60
                                                                        .04500
'RB'37. 085.5 15.200 01.810 0495 00.00 1.0000 0.692 00.927 00.827 07.318 235.500
    2.68 00.816 033.90 2.73 05.998 028.80 06.643 020.80 006.89 006.10
                                                                        .04625
'SR'38. 087.6 16.110 01.940 0510 00.00 1.0000 0.718 00.876 00.781 06.863 251.300
    2.68 00.770 036.50 2.73 05.583 031.20 06.172 022.40 06.387 006.62
                                                                        .04750
' Y'39. 088.9 17.040 02.080 0524 00.001.0000  0.744 00.830 00.738 06.449 268.100
    2.67 00.728 039.30 2.73 05.232 033.50 05.755 024.10 05.961 007.18
                                                                        .04875
'ZR'40. 091.2 00.000 02.220 0538 00.00 0.5000 0.770 00.787 00.700 06.070
                042.30 2.73 04.867 036.15 05.378 025.95 05.538 007.78
                                                                        .05000
'NB'41. 092.9 00.000 02.370 0553 00.00 1.0000 0.796 00.746       05.724
                045.50 2.73 04.581 038.90 05.026 027.90 05.223 008.39
                                                                        .05600
```

TABLE I—(continued)

```
FL  NO. WGT.- VC(K)- VC(L)- -J-- -RK-- -OXY-- OMGAK KALPHA KBETA- LALPHA --CK---
    -NK- KFDGF- --CKL- NKL- --L1-- -CL1-- --L2-- -CL2-- --L3-- -CLM-- --M1--
    -CM1- -M2--- CM2- --M3-- CM3- --M4-- --M5-- CMN-- --N1-- OMGAL

'MO'42. 096.0 00.000 02.520 0567 00.00 1.0000 0.822 00.710          05.406
                048.50 2.72 04.298 041.45 04.718 029.75 04.913 009.05
                                                                    .062
'TC'43. 099.0 00.000 02.680 0581 00.00 1.0000 0.848                00.000
                052.10 2.72 04.060 044.50 04.436 031.95 04.632 009.74
                                                                    .068
'RU'44. 101.7 00.000 02.840 0595 00.00 1.0000 0.874                04.846
                055.60 2.72 003.83 047.50 04.180 034.10 04.369 010.47
                                                                    .074
'RH'45. 102.9 00.000 03.000 0609 00.00 1.0000 0.900                04.597
                059.30 2.72 03.626 050.70 03.942 036.40 04.130 011.24
                                                                    .080
'PD'46. 106.4 00.000 03.170 0623 00.00 1.0000 0.926                04.368
                063.10 2.72 03.428 053.95 03.724 038.70 03.908 012.03
                                                                    .086
'AG'47. 107.9 00.000 03.350 0637 00.00 2.0000 0.952                04.154
                067.30 2.71 03.254 057.50 03.514 041.30 03.698 012.87
                                                                    .092
'CD'48. 112.4 00.000 03.540 0651 00.00 1.0000 0.978                03.956
                071.00 2.71 03.085 060.70 03.326 043.60 03.504 013.76
                                                                    .098
'IN'49. 114.8 00.000 03.730 0665 00.00 1.0000 1.004                03.772
                075.50 2.71 02.926 064.50 03.147 046.30 03.324 014.68
                                                                    .104
'SN'50. 118.7 00.000 03.930 0679 00.00 1.0000 1.030                03.600
                079.60 2.71 02.777 068.00 02.982 048.80 03.156 015.65
                                                                    .110
'SB'51. 121.8 00.000 04.130 0692 00.00 0.6667 1.056                03.439
                084.20 2.70 02.639 071.95 02.830 051.70 3.0000 016.66
                                                                    .116
'TE'52. 127.6 00.000 04.340 0706 00.00 1.0000 1.082                03.289
                088.50 2.70 02.511 075.65 02.687 054.30 02.855 017.72
                                                                    .122
' I'53. 126.9 00.000 04.560 0720 00.00 1.0000 1.108                03.148
                094.00 2.70 02.389 080.35 02.553 057.70 02.719 018.82
                                                                    .128
'XE'54. 131.3 00.000 04.780 0734 00.00 1.0000 1.134                00.000
                098.30 2.69 02.274 084.00 02.429 060.30 02.592 019.97
                                                                    .134
'CS'55. 132.9 00.000 05.010 0747 00.00 1.0000 1.160                02.892
                103.40 2.69 02.167 088.40 02.314 063.40 02.474 021.16 10.202
    018.2                                                           .140
'BA'56. 137.4 00.000 05.250 0761 00.00 1.0000 1.186                02.775
                109.00 2.69 02.068 093.15 02.204 066.90 02.363 022.41 09.557
    019.3 10.845 16.0                                               .146
'LA'57. 138.9 00.000 05.480 0775 00.00 1.0000 1.212                02.665
                114.40 2.68 01.973 097.80 02.103 070.20 02.258 023.70 09.042
    020.4 10.321 16.9                                               .152
'CE'58. 140.1 00.000 05.72  0788 00.00 0.6667 1.238                02.561
                120.00 2.68 01.889 102.50 02.011 073.60 02.164 025.05 08.614
    021.6 09.692 17.9 10.408 15.5                                   .158
'PR'59. 140.9 00.000 05.960 0802 00.00 1.0000 1.264                02.463
                125.50 2.68 01.811 107.30 01.924 77.000 02.077 026.47 08.188
    022.8 09.258 18.9 09.957 16.3                                   .164
'ND'60. 144.3 00.000 06.210 0815 00.00 1.0000 1.290                02.370
                132.00 2.67 01.735 112.80 01.843 81.000 01.995 027.93 07.831
    024.1 08.773 20.0 09.499 17.2                                   .170
'PM'61. 145.0 00.000 06.460 0829 00.00 1.0000 1.316                02.283
                138.50 2.67 01.665 118.50 01.767 085.00 01.918 029.44 07.510
    025.4 08.376 21.0 09.115 18.2                                   .176
```

TABLE I–(continued)

```
FL  NO. WGT.- VC(K)- VC(L)- -J-- -RK-- -OXY-- OMGAK KALPHA KBETA- LALPHA --CK---
    -NK- KEDGE- --CKL- NKL- --L1-- -CL1-- --L2-- -CL2-- --L3-- -CLM-- --M1--
    -CM1- -M2--- CM2- --M3-- CM3- --M4-- --M5-- CMN-- --N1-- OMGAL

'SN'62. 150.4 00.000 06.720 0843 00.00 1.0000 1.342                02.199
                143.50 2.67 01.599 122.50 01.703 088.00 01.845 031.01 07.178
   026.7 08.023 22.2 08.705 19.1                                    .182
'EU'63. 152.0 00.000 06.980 0856 00.00 1.0000 1.368                02.121
                150.00 2.66 01.536 128.00 01.626 092.00 01.775 032.63 06.856
   028.1 07.642 23.3 08.331 20.1 10.604 10.893 13.85                .188
'GD'64. 156.9 00.000 07.240 0870 00.00 1.0000 1.394                02.046
                157.00 2.66 01.477 134.00 01.561 096.30 01.710 034.31 06.566
  029.6 07.322 24.5 07.997 21.2 10.111 10.408 14.30                 .194
'TB'65. 158.9 00.000 07.520 0883 00.00 1.0000 1.420                01.975
                163.50 2.65 01.421 140.00 01.501 100.30 01.649 036.06 06.292
   031.1 07.011 25.8 07.685 22.3 09.692 09.957 14.80                .200
'DY'66. 162.5 00.000 07.790 0897 00.00 1.0000 1.446                01.909
                170.50 2.65 01.365 146.00 01.438 104.50 01.579 037.86 06.088
   032.6 06.715 27.0 07.383 23.4 09.258 09.528 15.30                .206
'HO'67. 164.9 00.000 08.070 0910 00.00 1.0000 1.472                01.845
                176.50 2.65 01.317 151.00 01.390 108.50 01.535 039.76 05.820
   034.3 06.453 28.5 07.128 24.5 08.899 09.155 15.85                .212
'ER'68. 167.2 00.000 08.360 0923 00.00 1.0000 1.498                01.784
                184.00 2.64 01.268 157.00 01.33, 113.00 01.482 041.69 05.581
   035.9 06.179 29.8 06.834 25.7 08.508 08.773 16.30                .218
'TM'69. 168.9 00.000 08.650 0937 00.00 1.0000 1.524                01.726
                192.50 2.64 01.222 165.00 01.288 118.00 01.433 043.69 05.366
   037.7 05.931 31.2 06.559 27.0 08.155 08.433 16.85                .224
'YB'70. 173.0 00.000 08.940 0950 00.00 1.0000 1.550                01.672
                199.00 2.63 01.182 170.00 01.243 122.00 01.386 045.79 05.161
   039.6 05.686 32.7 06.331 28.3 07.836 08.086 17.45                .230
'LU'71. 175.0 00.000 09.250 0964 00.00 1.0000 1.576                01.619
                206.00 2.63 1.1400 176.00 01.199 126.00 01.341 047.92 04.972
   041.3 05.475 34.2 06.112 29.6 07.545 07.777 18.00                .245
'HF'72. 178.6 00.000 09.560 0997 00.00 1.0000 1.602                01.570
                214.00 2.62 01.100 183.00 01.155 131.00 01.297 050.13 04.753
   043.2 05.211 35.8 05.861 30.9 07.190 07.427 18.55                .260
'TA'73. 180.9 00.000 09.880 0991 00.00 1.0000 1.628                01.522
                222.00 2.62 01.061 190.00 01.114 136.00 01.255 052.44 04.569
   045.2 05.015 37.5 05.627 32.4 06.898 07.128 19.05                .275
' W'74. 183.9 00.000 10.200 1004 00.00 1.0000 1.654                01.476
                231.00 2.61 01.025 197.00 01.075 142.00 01.216 054.79 04.405
   047.2 04.823 39.1 05.451 33.8 06.640 06.871 19.60                .290
'RE'75. 186.2 00.000 10.500 1017 00.00 1.0000 1.680
                239.00 2.61 00.990 204.00 01.037 147.00 01.177 057.21 04.231
   049.3 04.625 40.9 05.253 35.3 06.357 06.594 20.10                .305
'OS'76. 190.2 00.000 10.900 1031 00.00 1.0000 1.706                01.391
                247.00 2.60 00.956 211.00 01.001 152.00 01.140 059.70 04.064
   051.5 04.443 42.6 05.060 36.9 06.106 06.357 20.45                .320
'IR'77. 193.1 00.000 11.200 1044 00.00 1.0000 1.732                01.351
                256.00 2.60 00.923 219.00 00.967 157.00 01.106 062.27 03.915
   053.7 04.273 44.5 04.873 38.4 05.880 06.094 21.35                .335
'PT'78. 195.1 00.000 11.600 1057 00.00 1.0000 1.758                01.313
                263.00 2.59 00.893 225.00 00.934 161.00 01.072 064.92 03.774
  056.0 04.114 46.4 04.710 40.1 05.665 05.880 21.95                 .350
'AU'79. 197.2 00.000 11.900 1071 00.00 1.0000 1.784                01.276
                272.00 2.59 00.863 232.00 00.903 167.00 01.040 067.64 03.620
   058.3 03.939 48.3 04.522 41.8 05.415 05.629 22.50                .365
'HG'80. 200.6 00.000 12.300 1084 00.00 1.0000 1.810                01.241
                281.00 2.58 00.835 240.00 00.872 172.00 01.008 070.55 03.482
   060.8 03.779 50.4 04.349 43.6 05.280 05.413 23.10                .380
'TL'81. 204.4 00.000 12.600 1097 00.00 1.0000 1.836                01.207
                289.00 2.58 00.808 247.00 00.843 177.00 00.979 073.60 03.349
    063.5 03.632 52.6 04.201 45.4 04.998 05.200 23.80               .385
```

TABLE I–(Continued)

```
FL  NO. WGT.- VC(K)- VC(L)- -J-- -RK-- -OXY-- OMGAK KALPHA KBETA- LALPHA --CK---
    -NK- KEDGE- --CKL- NKL- --L1-- -CL1-- --L2-- -CL2-- --L3-- -CLM-- --M1--
    -CM1- -M2--- CM2- --M3-- CM3- --M4-- --M5-- CMN-- --N1-- OMGAL

'PB'82. 207.2 00.000 13.000 1111 00.00 1.0000 1.862                  01.175
                298.00 2.57 00.782 255.00 00.815 183.00 00.950 076.64 03.218
    066.1 03.484 54.7 04.042 47.3 04.797 04.994 24.40          .390
'BI'83. 209.0 00.000 13.400 1124 00.00 0.6667 1.888                  01.144
                307.00 2.56 00.757 262.00 00.789 188.00 00.923 079.94 03.099
    068.9 03.355 57.1 03.902 49.3 04.612 04.808 25.10          .395
'TH'90. 232.1 00.000 16.300 1217 00.00 1.0000 2.070                  00.956
                                                  00.761 109.40 02.401
    094.3 02.577 78.1 03.080 67.5 03.573 03.745 31.30 9.492   .430
' U'92. 238.1 00.000 17.200 1244 00.00 1.0000 2.122                  00.911
                                                  00.722 120.70 02.235
    104.0 02.394 86.2 02.882 74.5 03.300 03.496 33.60 8.614   .440
```

The order in which the Element File is used as input is most important. If we run in MODE = 1, the order of the element cards as submitted to the computer, must be the same as the order in which the probe measured the elements; for example, if data set 1 consisted of elements E_1, E_2, E_3, measured on spectrometers 1, 2, and 3, respectively, and set 2 consisted of E_4, E_5, measured on spectrometers 1 and 2 respectively, then the order of the element cards must be E_1, E_2, E_3, E_4, E_5. If other elements are present in the unknown and their weight percentages are known, their element cards come next. If oxygen is present in the unknown, its element cards are next. The last elements considered in the Element File are the file cards of elements present in the standards but not in the unknown. The element file is input following the DATA File. Figure 9 shows data for Input Files A and B for one of the sample problems (Appendix VI).

C-Composition Files

The composition file consists of the following types of data:

(1) Title card for the unknown sample. On this card may be punched up to 80 characters of alphanumeric information to aid the experimenter in identifying his problem. This information is stored in the UTITLE array. The statement in MAIN;

Read (IN,40) (UTITLE(I), I = 1,20) accomplishes the data transmittal.

(2) Composition card(s) for the unknown sample. The composition of each element in the unknown (wt. %), if known before the analysis, is input here. If it is not known it is set to zero. For example in columns 1-10 is punched the weight % of E(1) present in the unknown; in columns 11-20, the weight % of

E(2), . . ., in columns 71-80, the weight % of E(8). On the second card in columns 1-10 goes the weight % of E(9), and so forth, until the weight percentage of each of the NEU elements in the unknown, if available before electron probe analysis, has been entered ($1 \leq NEU \leq 10$). Note: The order of the elements in the unknown should be the same as in the E list. If none of the sample compositions is known, they are all set to zero. The statement in MAIN

```
READ (IN,2)  (C(I), I = 1, NEU)
```

2 FORMAT (8F10.2), accomplishes the data transmittal.

(3) Cards for the Standards. These cards are input using the following statements:

```
DO  600 K = 1, NM
READ (IN,40) (STITLE(I,K), I = 1,20)
READ (IN,41) NEST, (ESTD(I,K), I = 1, NEST)
READ (IN,2) (CS(I,K), I = 1, NEST)
600 CONTINUE
```

The first READ inputs the title card for standard #K. The second READ inputs the second card which contains the number of elements in standard #K and the chemical symbols of each of these elements. On this card columns 1-4 contain the number of elements, 5--8, the name of ESTD (1,K), 9-12, the name of ESTD (2,K), ..., 41-44, the name of ESTD (10,K). All entries on this card must be right-adjusted. The third READ statement inputs the next cards which give the wt. % of ESTD (1, K), ..., ESTD(NEST,K), respectively. The same format (8F10.2), as that used to input any known compositions in the unknown sample, is also used here. The order of the standards, K = 1, 2, . . ., NM, must be the order in which their intensities were measured. Thus, if STANDARD #12 was measured first, then information regarding it will be found whenever K = 1; if STANDARD #10 read second, then information regarding it stored for K = 2.

(4) Cards for the backgrounds. If NBGS > 0, then for each background standard a title card of identifying information is input. This is accomplished by the statements in MAIN:

```
DO 800 K = 1, NBGS
800    READ (IN,40) (BTITLE(I,K), K = 1,20).
```

Figure 10 shows data from the Composition File as used in the sample problem illustrated in Appendix VI.

D-Intensity Data File

Whenever the program is operating in MODE 1, subroutine DATPTS inputs D. The following procedure may have to be changed according to the type of output data obtained from each particular electron probe. The type of identification scheme used at GSFC is outlined here. To change the scheme, DATPTS, Appendix III, may have to be reprogrammed.

Each probe measurement is recorded on a punched card, which is divided into 10 fields. These fields contain

(1) the x-ray counting time (TIME)

(2-4) the intensity counts for each spectrometer (XINT(I)), I = 1,2,3)

(5) the sample-type code (SAME) for unknown, standard, or background,

(6) the set-number (NUMRDG), which tells whether element group 1 (E(1) - E(3)), 2 (E(4)-E(6)) or 3 (E(7)-E(9)) is being measured

(7) the group - number (INDIC) which tells the number of times the standards, as a group, have been measured. INDIC is used so that the drift calculation can be made several times during a run

(8) the number or identification of the standard or background being measured (NOST). As discussed in the description of the Composition File, the background and standards are remembered according to the order in which their intensities were measured (1,2,3. . . .). Therefore this realignment is used for NOST

(9) the dummy variable (IUNK) for unspecified usage,

(10) the end of data card (LAST). This field is used on the last data card of a problem to indicate the end of the data. Its usage allows a second problem to be run.

The statements:

READ(IN,1) TIME, (XINT(J), J = 1,3), SAME, NUMRIDG, INDIC, NOST, IUNK, LAST

1 FORMAT (F6.0, 3F8.0, 4I1, I2,I1)

input one card. The data are then processed according to the value of SAME. Table II presents a capsule review of the use of the 10 fields with some additional comments.

TABLE II
Format for Intensity Data File

Field	Columns	Format	Parameter	Comment
1	1-6	F6.0	TIME	duration of measurement
2	7-14	F8.0	XINT(1)	intensity in counts from spectrometer #1
3	15-22	F8.0	XINT(2)	intensity from spectrometer #2
4	23-30	F8.0	XINT(3)	intensity from spectrometer #3
5	31	I1	SAME	SAME = 1 unknown measured SAME = 2 standard measured SAME = 3 background measured
6	32	I1	NUMRDG	NUMRDG = 1 measurements taken on E(1),E(2),E(3) (Set 1) NUMRDG = 2 measurements taken on E(4),E(5),E(6) (Set 2) NUMRDG = 3 measurements taken on E(7),E(8),E(9) (Set 3)
7	33	I1	INDIC	INDIC = i, i = 1,2,. . . ., 9 ith time readings are taken on standards
8	34	I1	NOST	NOST = i, i = 1,2,. . ., NM measurement taken on the ith standard
9	35-36	I2	IUNK	IUNK = i, i = 1, 2, ..., 99 Dummy variable for other usage
10	37	I1	LAST	LAST = 0 except on last data card where LAST = 1. This indicates the end of the data for the problem.

APPENDIX V
Output from the Program

The format of the data output and the FORTRAN statements which control this output are given below. The FORTRAN statements are referred to by their sequence numbers (SN) which appear to the right of each statement in the program listing (Appendix I).

Data set B, that is the E file, and selected parameters from data set A are printed out by MAIN, SN 15200: 19700. The matrix of mass absorption coefficients is calculated in SUBROUTINE ABSCO, SN 6500: 8100. The raw probe data are output in SUBROUTINE DATPTS at SN 4700: 4900, SN 6200: 6300, SN 7100: 7200, according to whether the measurement was of an unknown, a standard, or a background, respectively. For each standard, the title and composition cards are printed by MAIN, SN 24100: 24300; and the atomic number correction is also printed by MAIN, SN 24400: 24400. For each element in each standard, the absorption correction is printed by MAIN, SN 25700: 25700 and the fluorescence correction is output in FLUCOR, SN 5200: 5300, SN 5800: 6200.

Whenever a new standard combination is used, a message is written by MAIN, SN 27500: 27500 telling which standard is used for each measured element in the unknown. The sample compositions are printed at each iteration step: MAIN, SN 32300: 32600 only for the first set of intensity data. The weight % sum is also printed out. No attempt is made to normalize the sum to 100%.

After the final iteration on the first data point in a MODE 1 problem and for MODE 2 problems, the atomic number corrections, the absorption corrections and the fluorescence corrections are printed by statements MAIN, SN 31000: 31600, FLUCOR, SN 5200: 5300, FLUCOR, SN 5800: 6200 respectively. For subsequent data points the compositions of the first and last iterations are written, MAIN 29200 and 32600. For MODE 2 problems intensity ratios are printed by MAIN, SN 33300: 33300. Sample output data are given in Appendix VI, where several sample problems are considered. The output format can be easily changed by altering the FORTRAN statements previously indicated.

APPENDIX VI
Sample Problems

Three sample problems will be described in order to illustrate the use of this program. A copy of the input data (Files A-D) and the output for each of the problems is supplied as a guide for the successful application of the program.

Problem 1 – (Geological Application)* A sample is analyzed in MODE 1 for the following 8 elements: Ca, Mg, Si, Al, Na, Mn, Cr, and Fe. Oxygen is also present as is 0.1 wt % Ti. Six standards are used: pure diopside for Ca, Mg and Si, and 5 other standards, one for Al, Na, Mn, Cr and Fe. The data were taken on an electron probe with 3 spectrometers and a takeoff angle of 52.5°. The operating voltage was 20 KV; only K lines were measured. Input Files A-C have already been illustrated (Figures 8-10). Input File D, the Intensity Data File, is shown in Figure 11. A shortened version of the Output Data is given in Figure 12.

The initial estimate of the unknown composition using a linear relation (Equation 15) is given in Table III as well as the final calculated compositions determined after 3 iterations.

TABLE III
Calculated Compositions Problem 1

Element	Initial Estimate (wt. %)	Final calculated composition (wt. %)
Ca	11.54	11.57
Mg	12.55	12.87
Si	25.13	26.1
Al	1.15	1.08
Na	0.88	0.93
Mn	0.09	0.09
Cr	0.59	0.58
Fe	2.57	2.59
Ti(known)	0.10	0.10
O	43.78	45.0
Sum	98.4	100.9

For all elements measured in this problem, the only correction factor of any significance was the absorption correction.

*This problem was kindly loaded to us by Dr. J. Boyd of the Geophysical Lab., Washington, D.C.

Problem 2 – (Metallurgical Application)* A binary sample is analyzed in MODE 1 for Ti and Nb only. Pure standards of the elements are used. The data was taken on an electron probe with 2 spectrometers and a takeoff angle of 52.5°. The operating voltage was 20 KV and Ti-K and Nb-L radiations were measured. Input Files A-D are illustrated in Figure 13 and the Output Data is given in Figure 14.

The initial estimate of the unknown composition using a linear relation (Equation 15) is given in Table IV as well as the final calculated composition determined after 3 iterations.

TABLE IV
Calculated Composition Problem 2

Element	Initial Estimates (wt. %)	Final Calculated Composition (wt. %)
Ti	32.7	34.8
Nb	62.2	65.5
Sum	94.9	100.3

For Ti, an atomic number correction of +7.6% is necessary while for Nb a negative atomic number correction of 5% is calculated. A significant absorption correction (~13%) was calculated for the Ti. The absorption correction for Nb was insignificant.

Problem 3 – (Metallurgical Application) A sample containing 4 elements has the following composition Al-10 wt. %, Mg-50 wt. %, Au-40 wt. %, Cu-0.10 wt. %. It is of interest to calculate using MODE 2 the expected concentration ratios (I /I(A)) for the 4 elements if pure standards of each element are used. The data is calculated for an electron probe with a takeoff angle of 52.5° and an operating voltage of 20 KV. The following x-ray lines were considered Al-K, Mg-K, Au-L and Cu-K. Input Files A-C are illustrated in Figure 15 and a shortened version of the Output Data is given in Figure 16.

The calculated intensity ratios are given in Table V.

This particular combination of elements exhibits a large atomic number effect (up to 30%) and a large absorption effect (up to 50%). Only Cu is noticeably fluoresced, namely by the Au-L line. Large corrections of this order, compounded with $f(\chi)$ values less than 0.8 for Al and Mg, argue quite strongly for the use of intermediate, 4 element, standards.

*This problem was kindly loaned to us by D. Beaman of the Dow Chemical Company, Midland, Michigan.

TABLE V
Calculated Intensity Ratios, Problem 3

Element	Composition (wt. %)	ANC = ATN/ATD	ABS = ABN/ABD	FLU = FLN/FLD	Intensity Ratio, Sample to Standard = ANC·ABS·FLU·C(U)
Al	10	1.14	0.48	1.0	5.5×10^{-2}
Mg	50	1.17	0.69	1.0	$41. \times 10^{-2}$
Au	40	0.71	1.01	1.0	$29. \times 10^{-2}$
CU	0.1	0.95	0.98	1.07	$.101 \times 10^{-2}$

APPENDIX VII

Figures

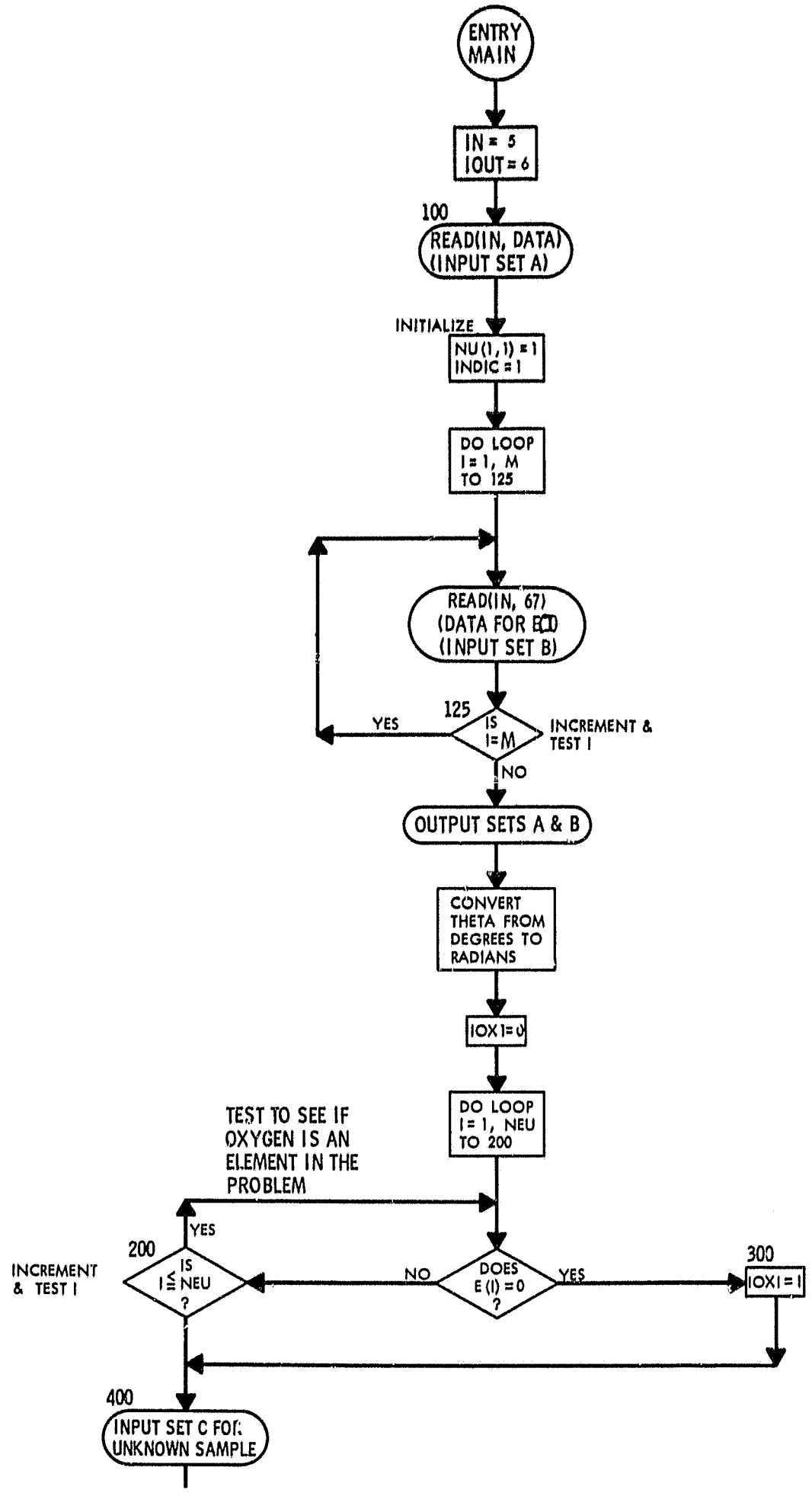


FIGURE 1 : MAIN PROGRAM

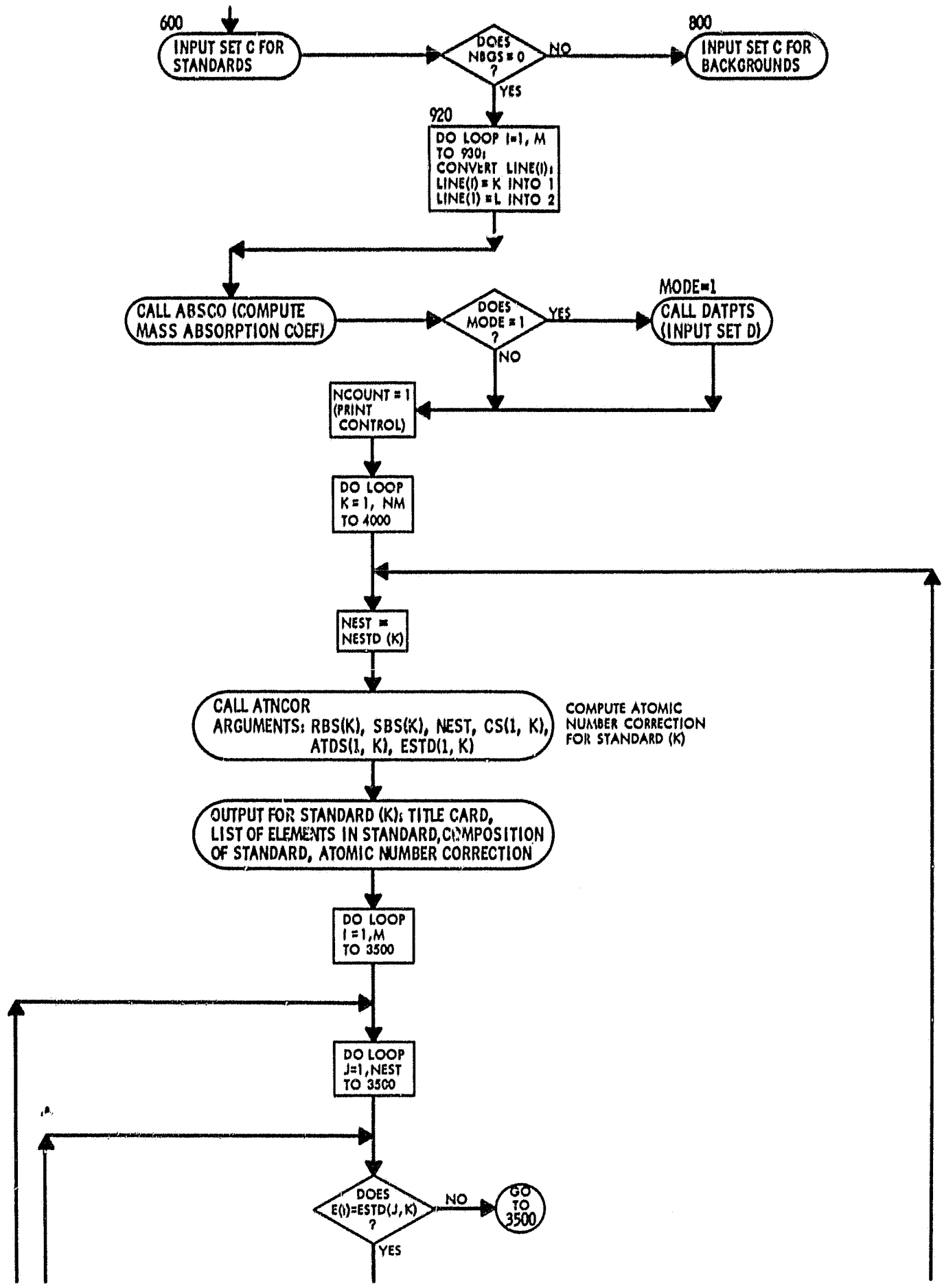


FIGURE 1 : MAIN PROGRAM (CONTINUED)

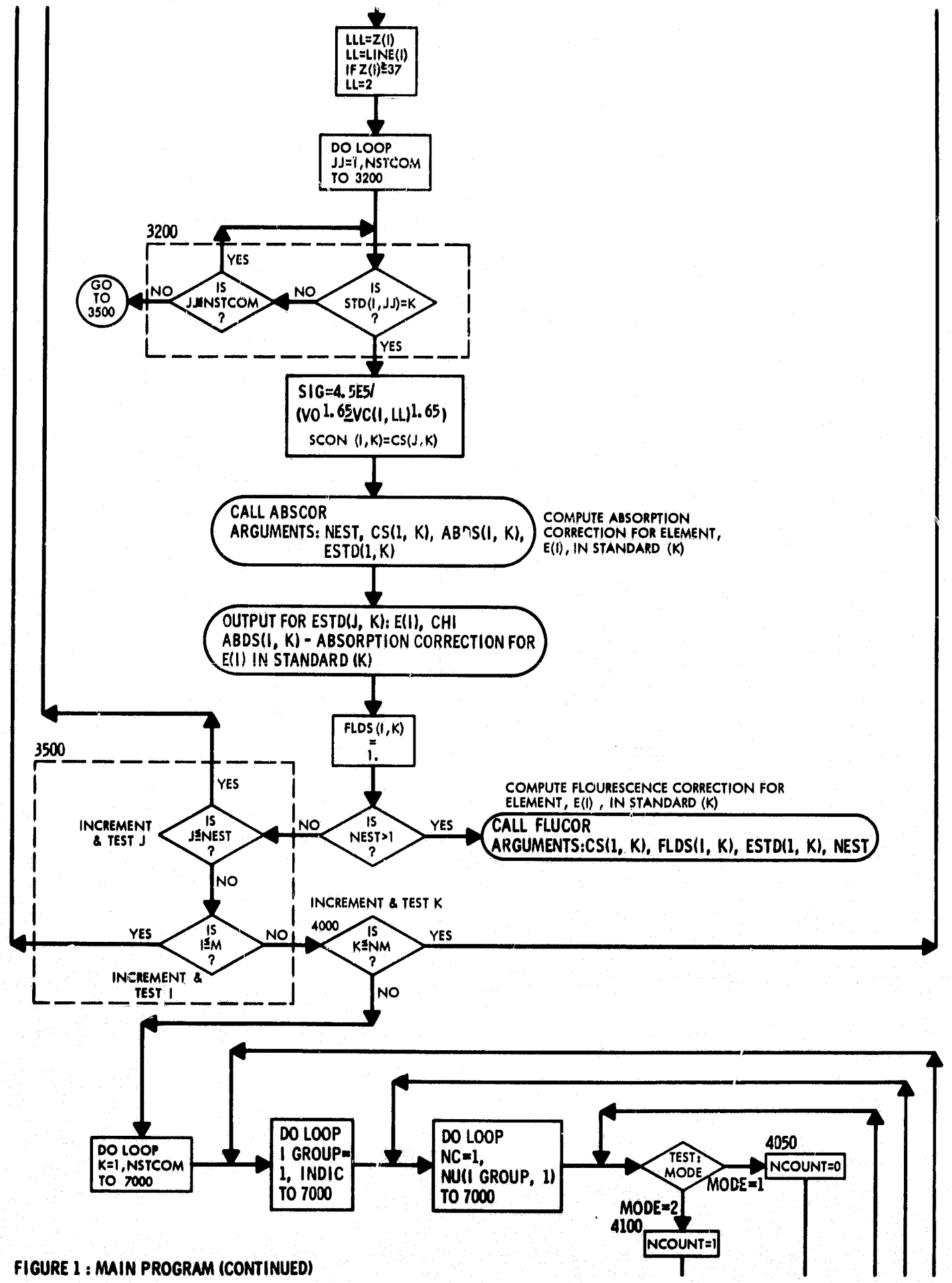


FIGURE 1 : MAIN PROGRAM (CONTINUED)

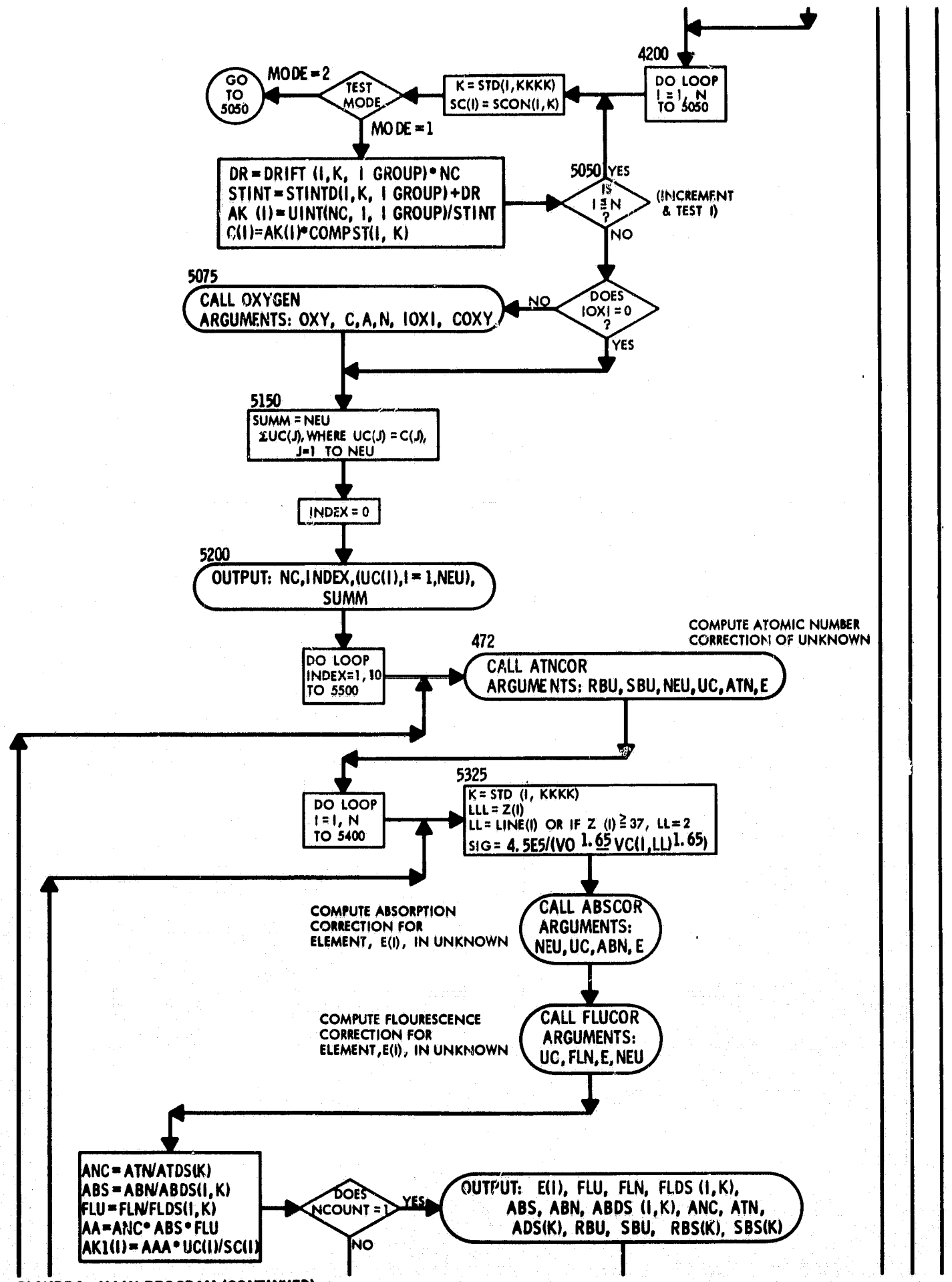


FIGURE 1 : MAIN PROGRAM (CONTINUED)

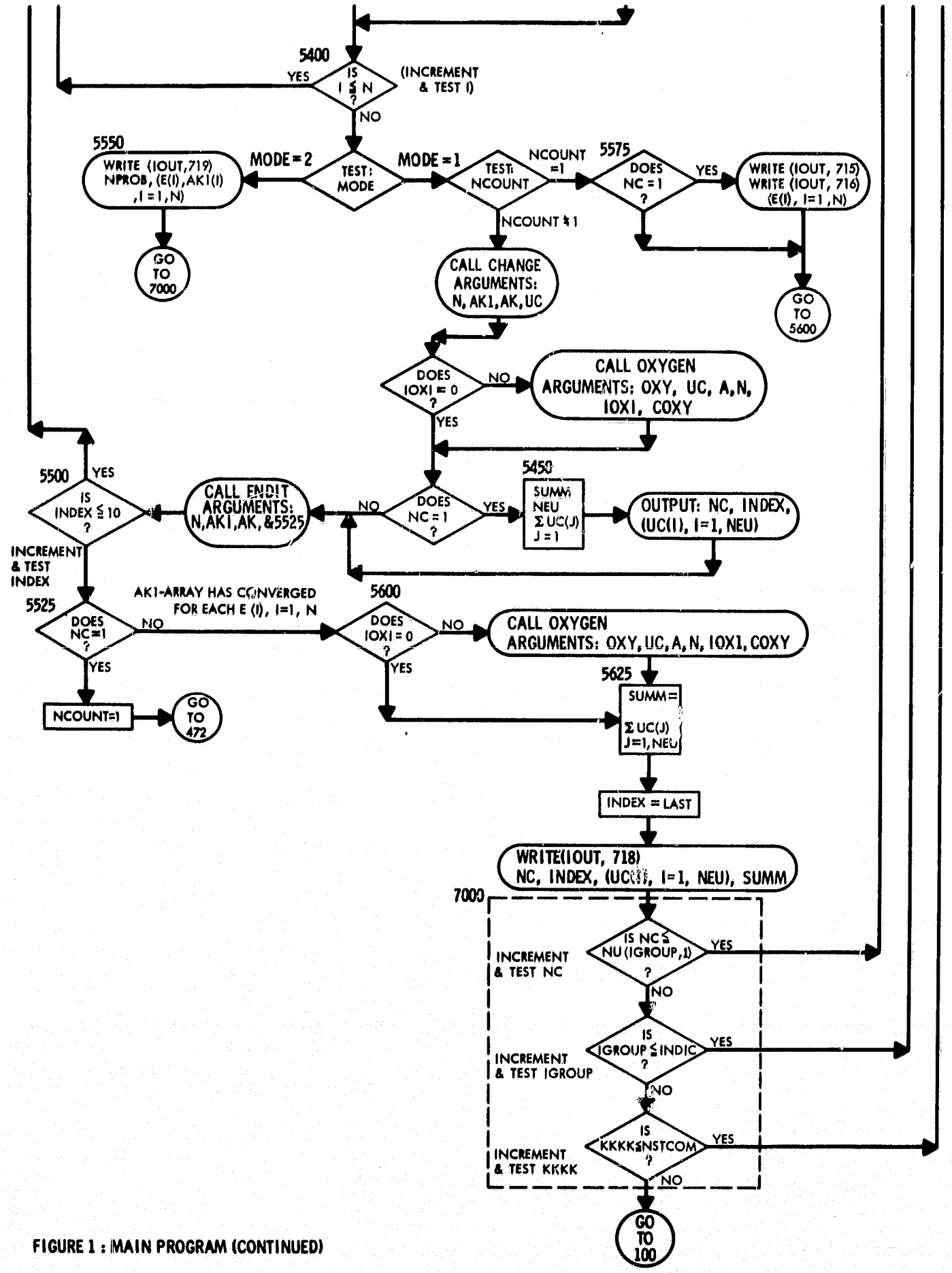


FIGURE 1 : MAIN PROGRAM (CONTINUED)

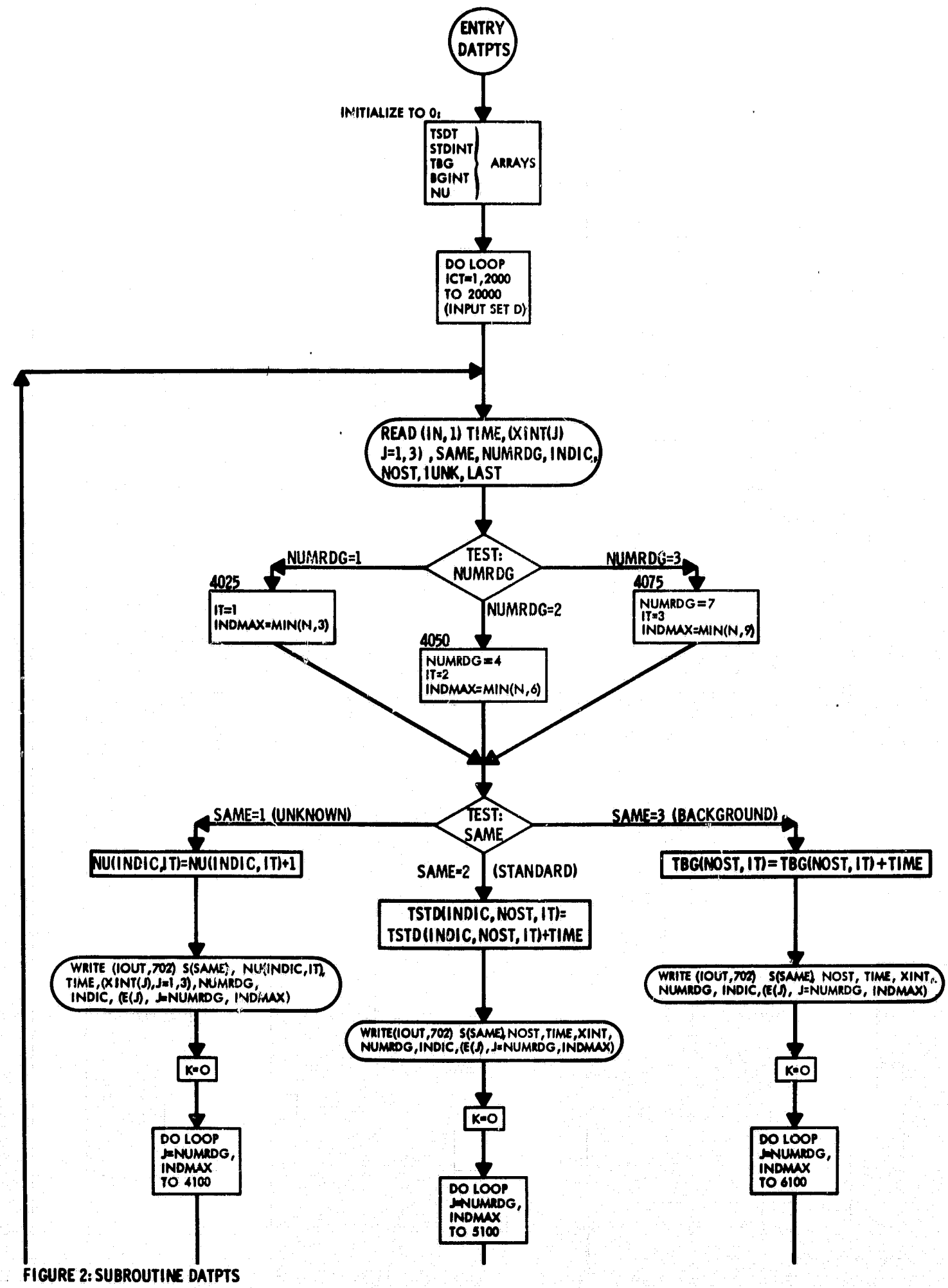


FIGURE 2: SUBROUTINE DATPTS

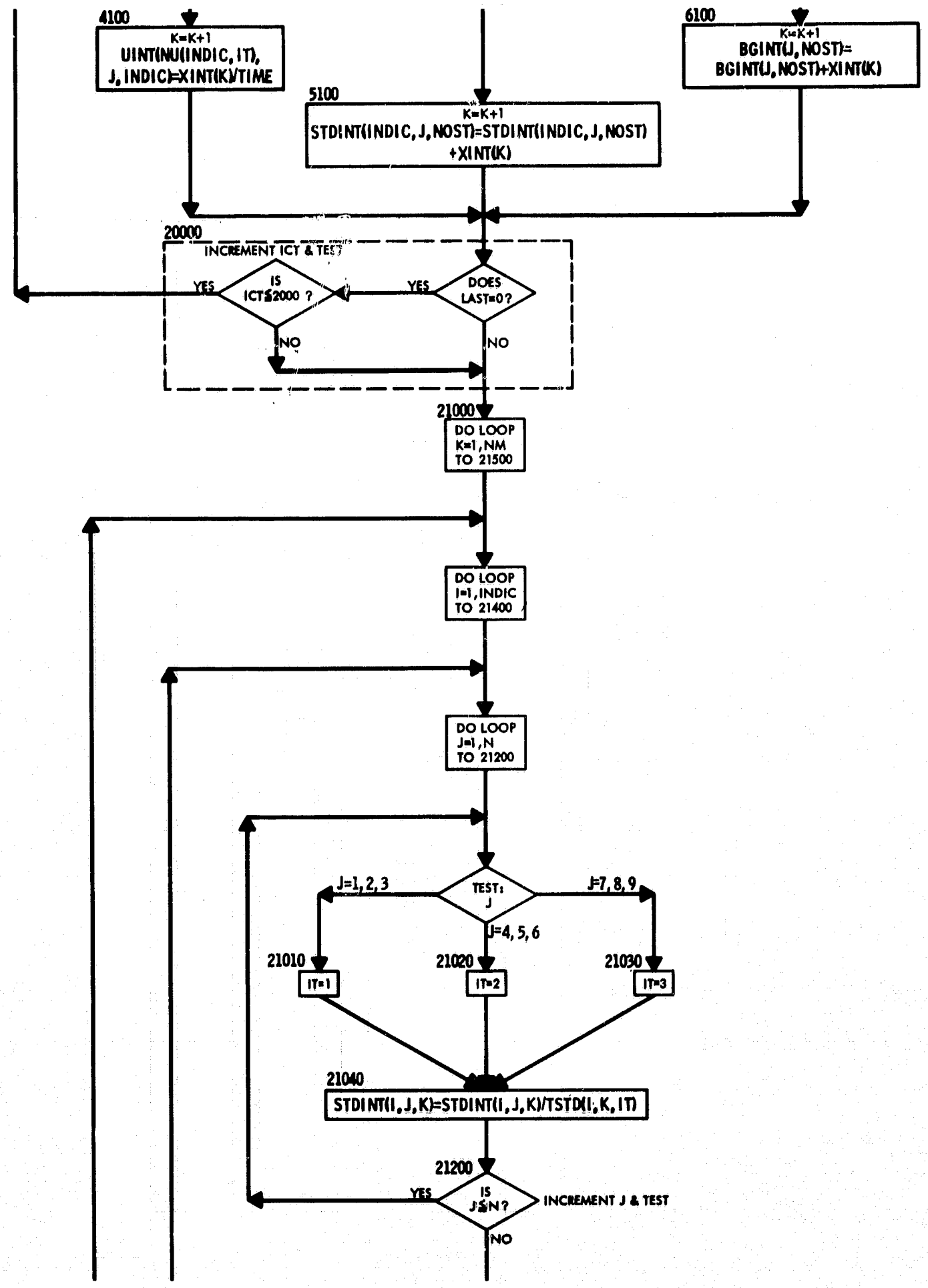


FIGURE 2 : SUBROUTINE DATPTS (CONTINUED)

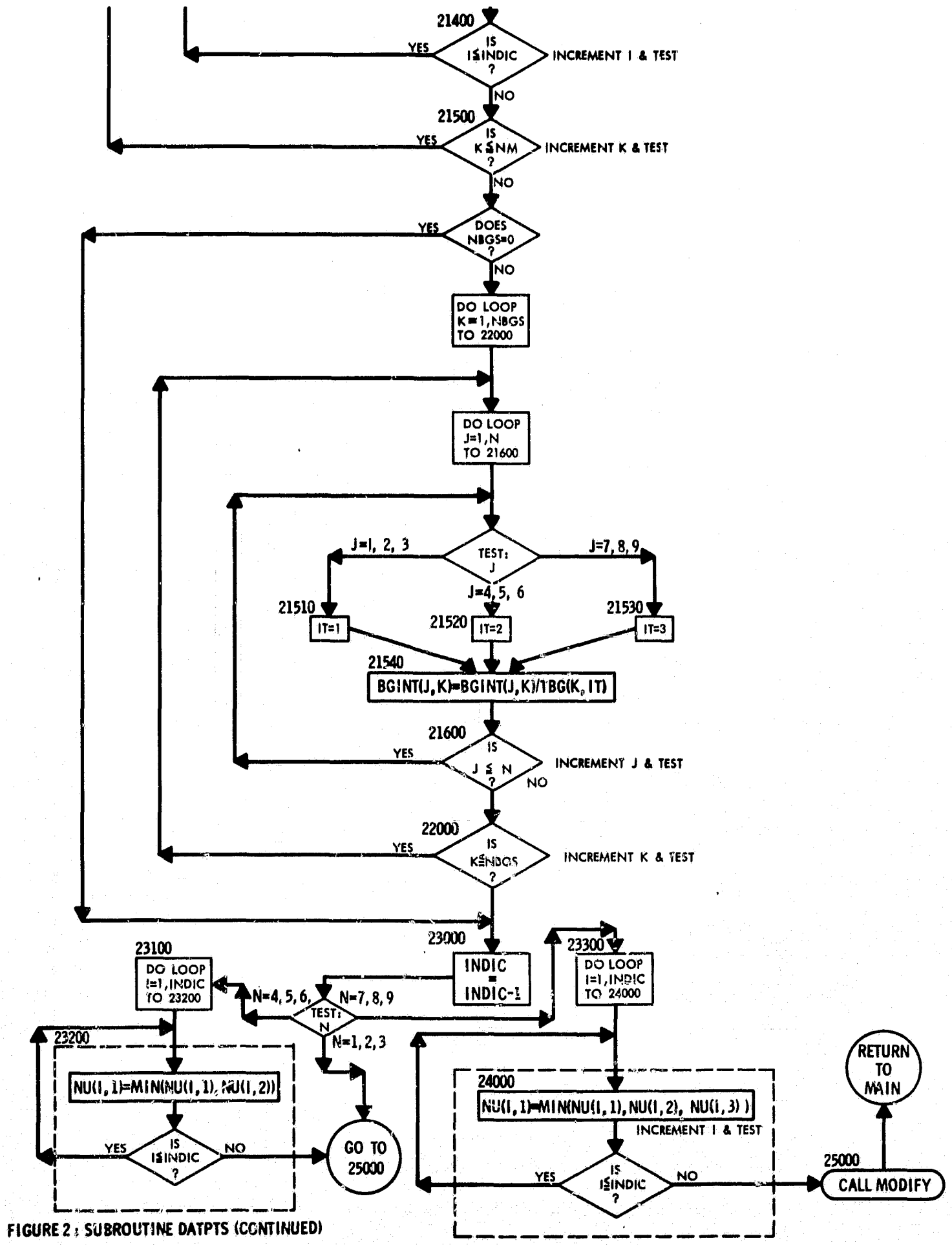
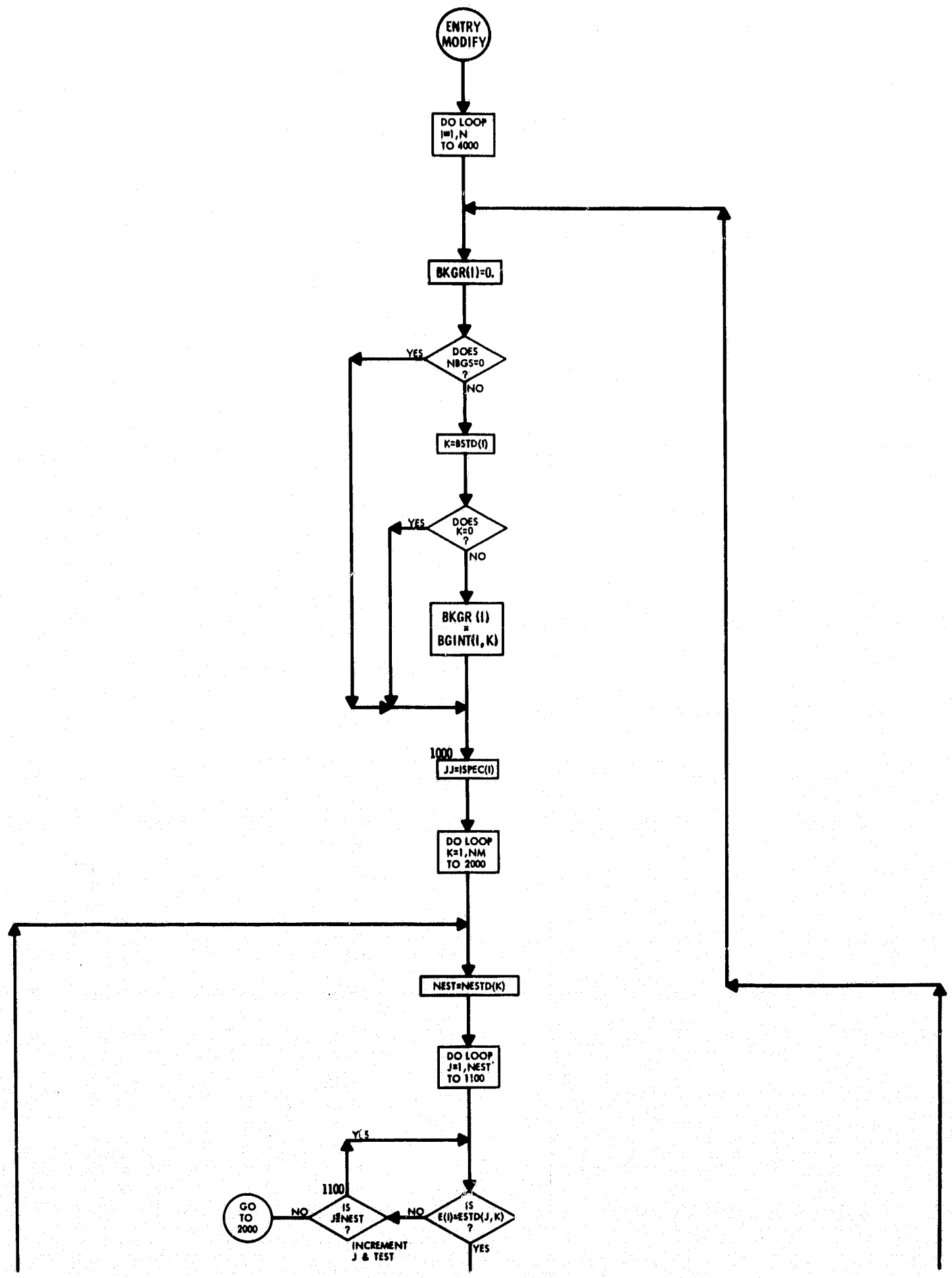


FIGURE 2 : SUBROUTINE DATPTS (CONTINUED)

FIGURE 3: SUBROUTINE MODIFY



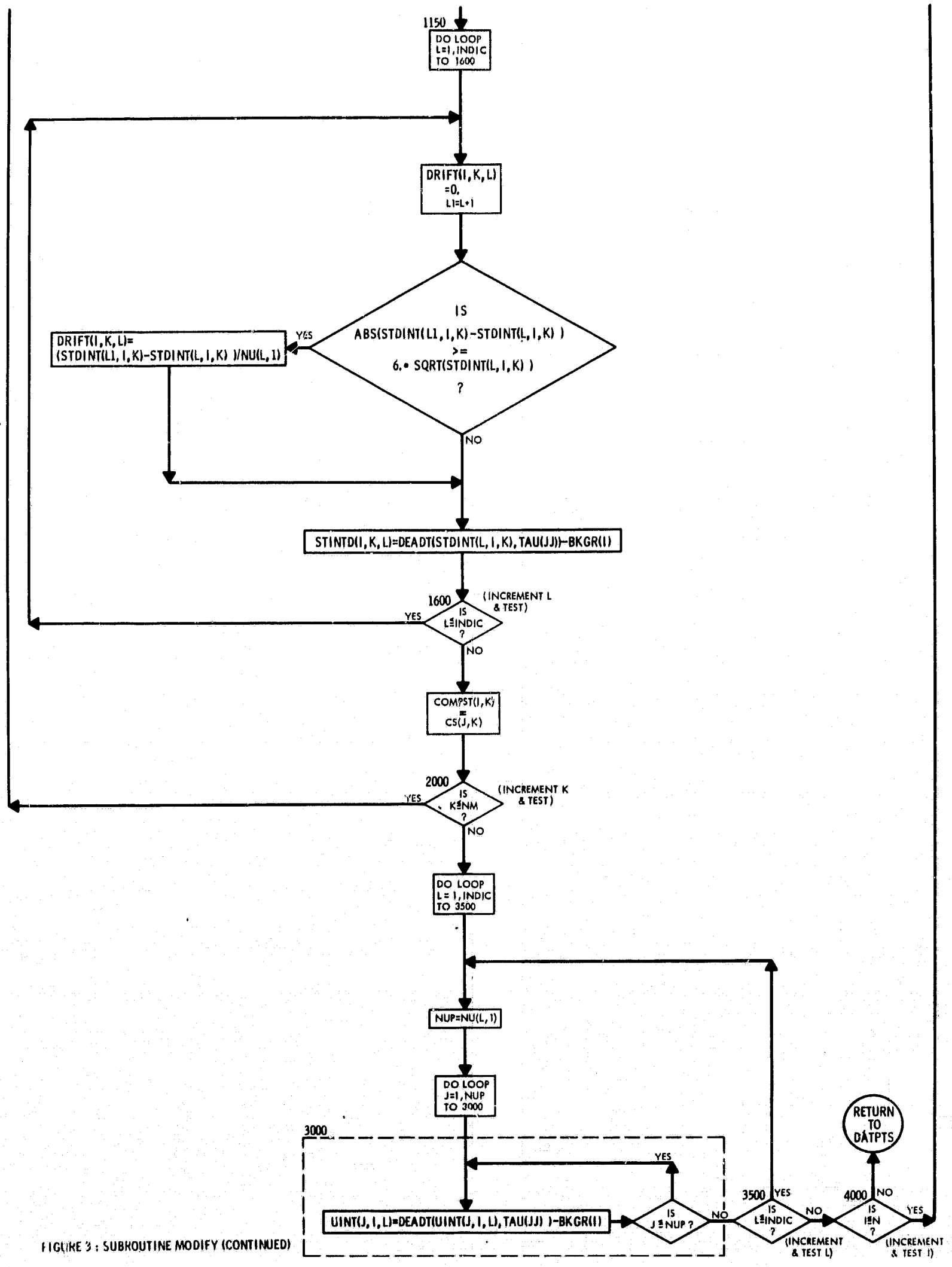


FIGURE 3 : SUBROUTINE MODIFY (CONTINUED)

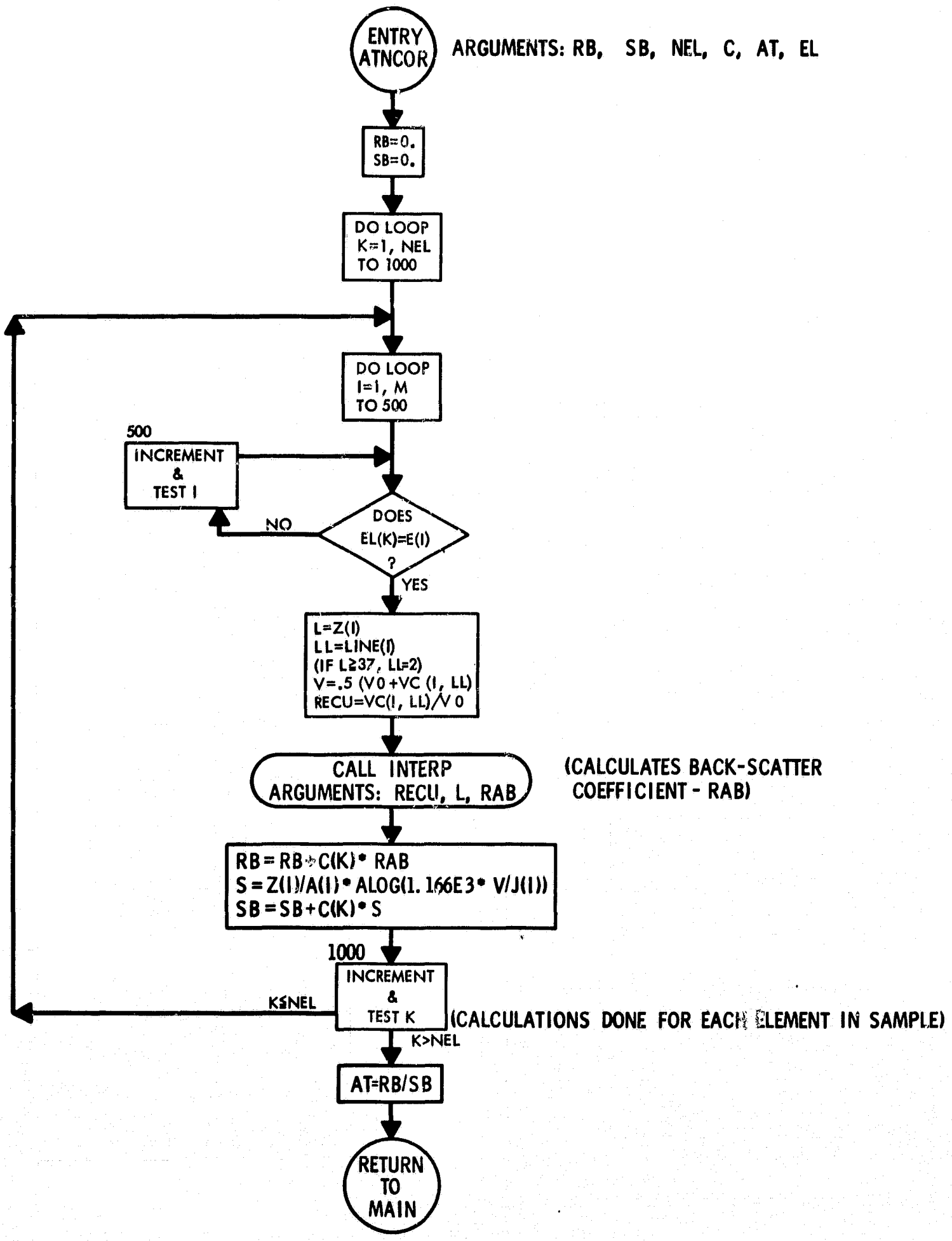


FIGURE 4: SUBROUTINE ATNCOR

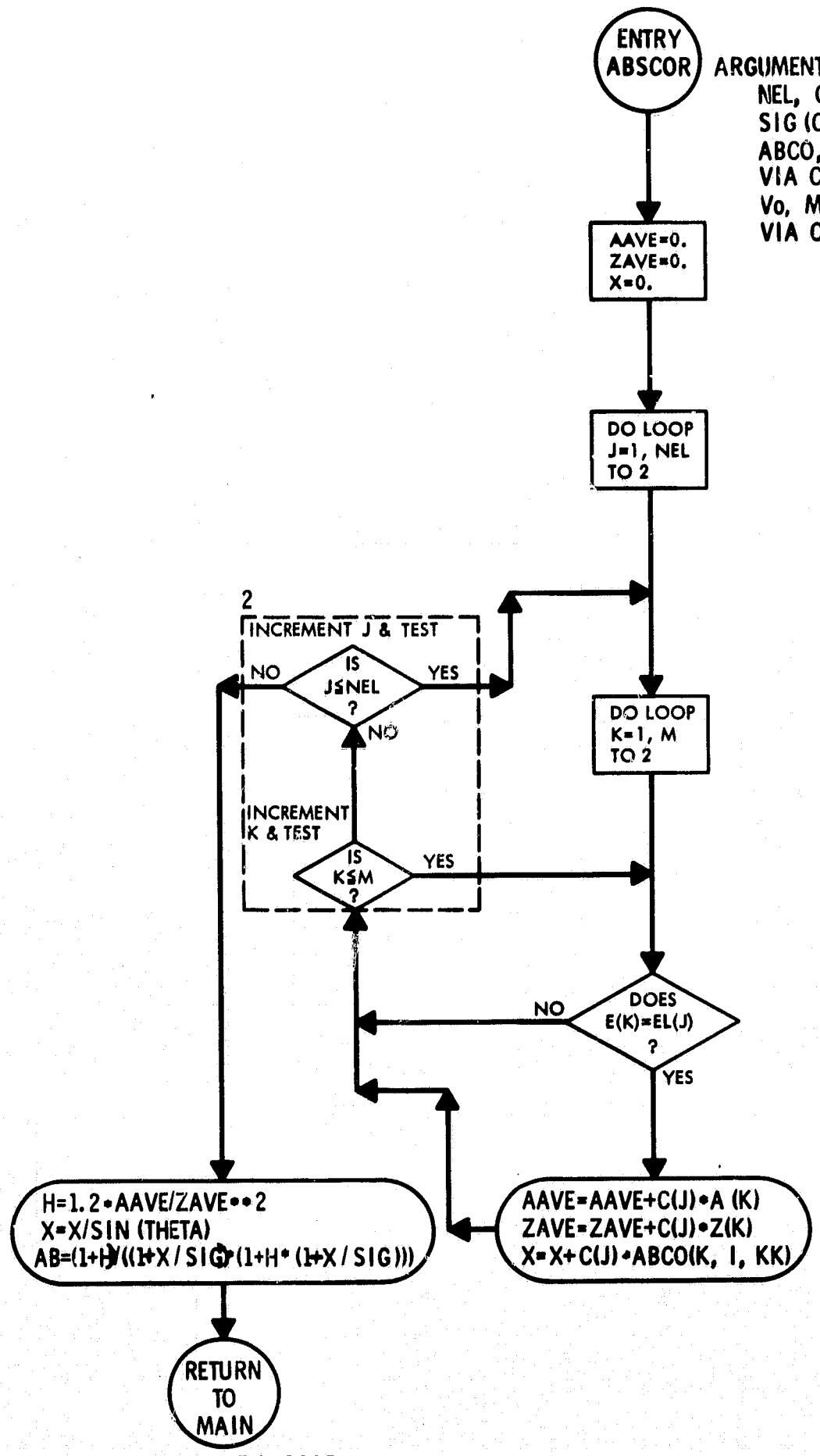


FIGURE 5: SUBROUTINE ABSCOR

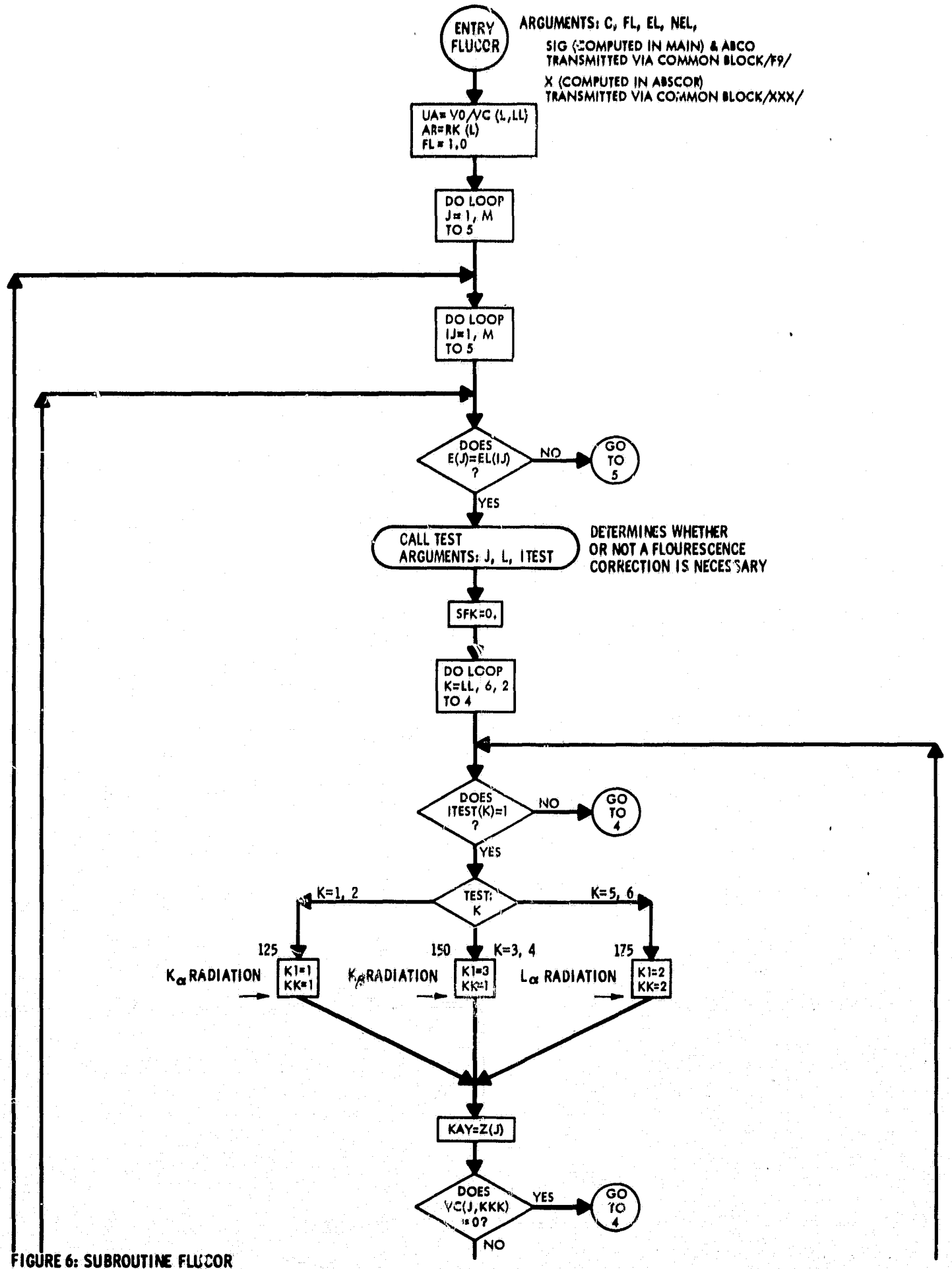


FIGURE 6: SUBROUTINE FLUCOR

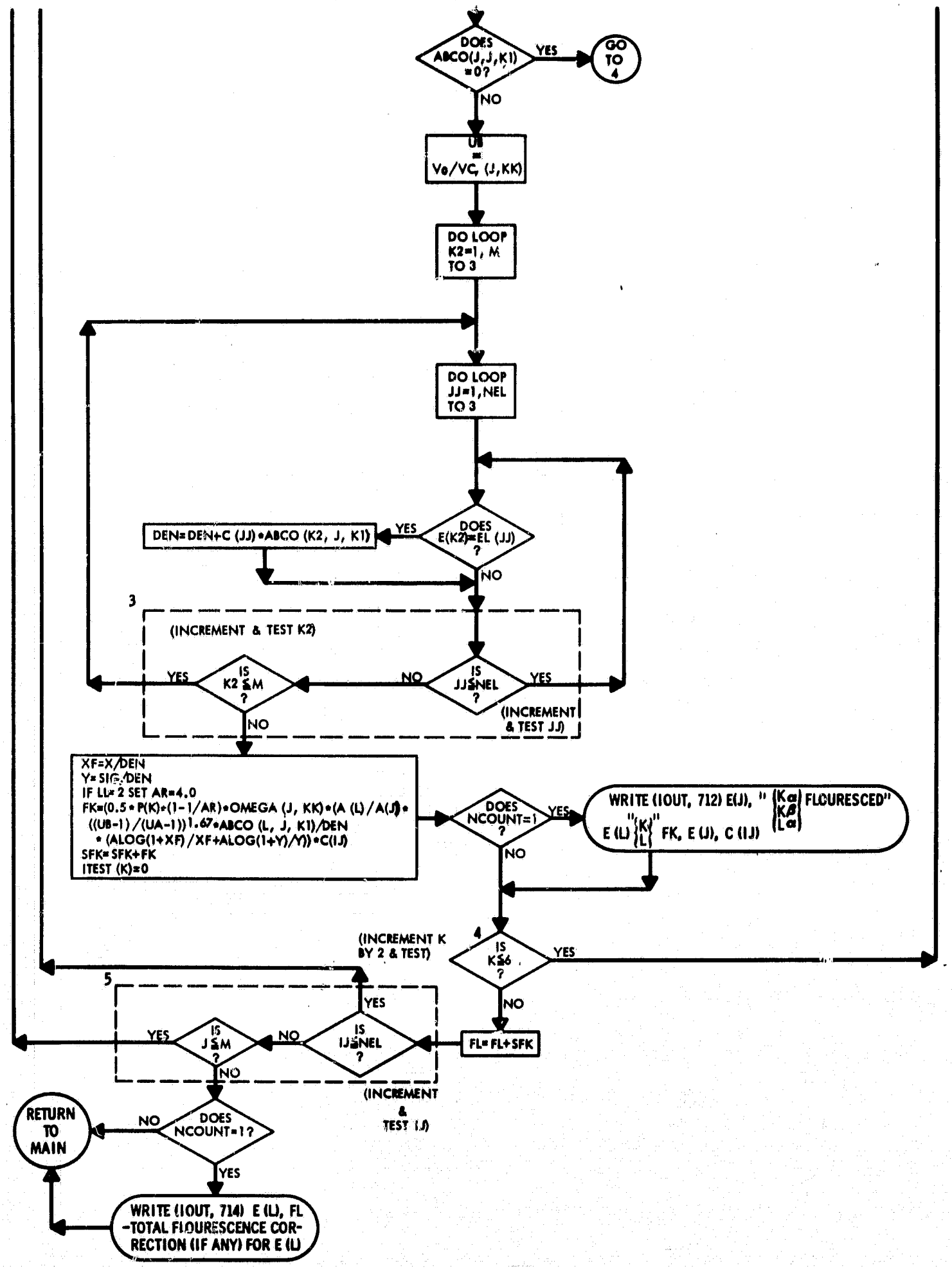
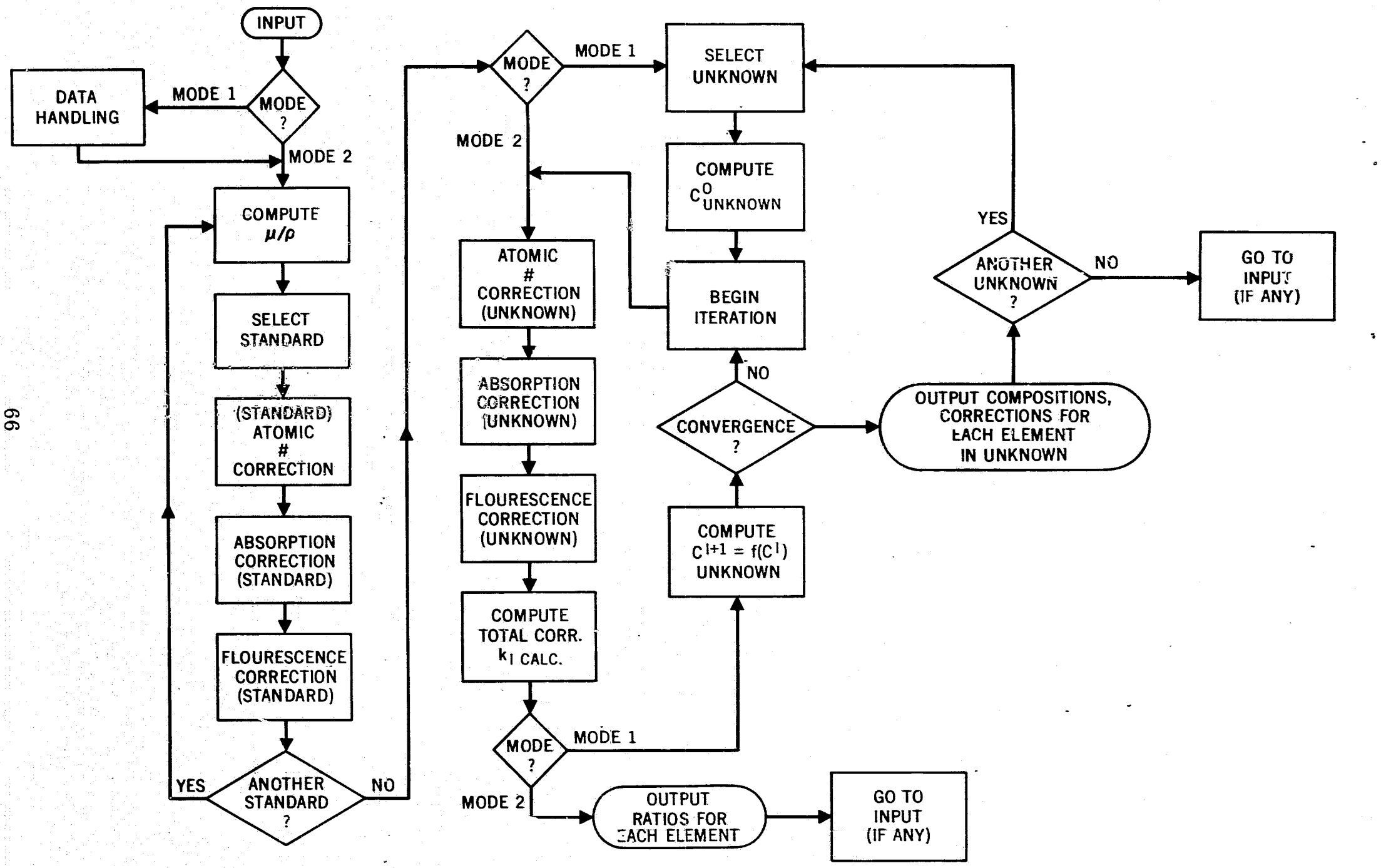


FIGURE 6 : SUBROUTINE FLUCOR (CONTINUED)

MICROPROBE CORRECTION PROGRAM



```
&DATA THETA=52.5,TAU=.15E-5,.30E-5,.15E-5,STD=3*1,2,3,4,5,6,82*0,
N=8,NEU=10,M=10,NM=6,NBGS=3,MODE=1,NPROB=2,NSTCOM=1,LINE=10*1K1,
ISPEC=1,2,3,1,2,3,1,2,0,BSTD=3*0,1,2*0,3,2,0,V0=20.0,
&END
```

Figure 8–Input Data – Sample Problem 1 – DATA Files

```
 &DATA THETA=52.5,TAU=.15E-5,.30E-5,.15E-5,STD=3*1,2,3,4,5,6,82*0,
 N=8,NEU=10,M=10,NM=6,NRGS=3,MODE=1,NPROB=2,NSTCOM=1,LINE=10*'K',
 ISPEC=1,2,3,1,2,3,1,2,0,BSTD=3*0,1,2*0,3,2,0,VO=20.0,
 &END
'CA'20. 040.1 04.040 00.349 0239 09.92 1.0000 0.180 03.359 03.090 36.330 048.400
    2.74 03.070 005.10 2.73                                          35.5
                                                                        .02500
'MG'12. 024.3 01.300 00.049 0133 12.35 1.0000 0.030 09.889 09.558 50.000 011.750
    2.79 09.512 000.89 2.73                                          250.7
                                                                        .01500
'SI'14. 028.1 01.840 00.100 0154 11.64 0.5000 0.056 07.126 06.768 50.000 018.500
    2.77 06.738 001.54 2.73                                          123.0
                                                                        .01750
'AL'13. 027.0 01.560 00.075 0142 11.99 0.6667 0.042 08.337 07.981 50.000 014.870
    2.78 07.951 001.18 2.73                                          170.4
                                                                        .01625
'NA'11. 023.0 01.070 00.000 0126 12.74 2.0000 0.020 11.910 11.617 50.000 009.050
    2.79 11.480 0.62   2.73
                                                                        .01375
'MN'25. 054.9 06.540 00.000 0316 08.83 1.0000 0.290 02.103 01.910 19.500 086.700
    2.72 01.896 010.45 2.73        8.85           5.9     19.1
                                                                        .03125
'CR'24. 052.0 05.990 00.598 0301 09.03 1.0000 0.268 02.291 02.085 21.640 078.000
    2.73 02.070 009.18 2.73 16.7   7.80   17.9    4.8     20.7
                                                                        .03000
'FE'26. 055.9 07.110 00.707 0332 08.64 1.0000 0.320 01.937 01.757 17.600 095.800
    2.72 01.743 011.75 2.73 17.2   10.0   17.2    7.0     17.525
                                                                        .03250
'TI'22. 047.9 04.970 00.450 0270 09.45 1.0000 0.224 02.748 02.514 27.420 062.100
    2.73 02.497 007.00 2.73                                          27.3
                                                                        .02750
' O' 8. 016.0 00.532 00.000 0127 14.08 1.0000 0.004 23.700 00.000 50.000 003.800
    2.82 23.320
```

Figure 9–Input Data – Sample Problem 1 – DATA and Element File

```
                                                                    .01000
 BOYD'S PROBLEM
0.          0.          0.          0.          0.          0.          0.          0.
0.1         .0334
 STANDARD #1.....PURE DIOPSIDE
   4  CA   MG   SI    O
18.51       11.23       25.93       44.33
 STANDARD #2.....ENAL 5
   4  MG   AL   SI    O
23.02       2.65        26.57       47.76
 STANDARD #3.....DJ 65 JD 35
   6  CA   MG   SI   NA   AL    O
12.03       7.30        26.59       3.98        4.67        45.16
 STANDARD #4.....PYROPE GLASS
   5  MN   MG   AL   SI    O
4.19        16.29       12.05       20.95       46.52
 STANDARD #5.....CR IN MD 75 GLASS
   5  CA   MG   CR   SI    O
13.62       14.20       1.31        25.93       44.94
 STANDARD #6.....P-140 FOSTERITE
   4  MG   FE   SI    O
31.04       5.66        19.27       44.03
 BACKGROUND FOR AL
 BACKGROUND FOR FE
 BACKGROUND FOR CR
```

Figure 10–Input Data – Sample Problem 1 – Composition File

```
&DATA THETA=52.5,TAU=.15E-5,.30E-5,.15E-5,STD=3*1,2,3,4,5,6,82*0,
N=8,NEU=10,M=10,NM=6,NRGS=3,MODE=1,NPROB=2,NSTCOM=1,IJNE=10*'K',
ISPEC=1,2,3,1,2,3,1,2,0,RSTD=3*0,1,2*0,3,2,0,V0=20.0,
&END
'CA'20. 040.1 04.040 00.349 0239 09.92 1.0000 0.180 03.350 03.090 36.330 048.400
    2.74 03.070 005.10 2.73                                          35.5
                                                                          .02500
'MG'12. 024.3 01.300 00.045 0133 12.35 1.0000 0.030 09.889 09.558 50.000 011.750
    2.79 09.512 000.89 2.73                                          250.7
                                                                          .01500
'SI'14. 028.1 01.840 00.100 0154 11.64 0.5000 0.056 07.126 06.768 50.000 016.500
    2.77 06.738 001.54 2.73                                          123.0
                                                                          .01750
'AL'13. 027.0 01.560 00.075 0142 11.99 0.6667 0.042 08.337 07.981 50.000 014.870
    2.78 07.951 001.18 2.73                                          170.4
                                                                          .01625
'NA'11. 023.0 01.070 00.000 0126 12.74 2.0000 0.020 11.910 11.617 50.000 009.050
    2.79 11.480 0.62   2.73
                                                                          .01375
'MN'25. 054.9 06.540 00.000 0316 08.83 1.0000 0.290 02.103 01.910 19.500 086.700
    2.72 01.896 010.45 2.73        8.85           5.9     19.1
                                                                          .03125
'CR'24. 052.0 05.990 00.598 0301 09.03 1.0000 0.268 02.291 02.085 21.640 078.000
    2.73 02.070 009.18 2.73 16.7   7.80   17.9   4.8     20.7
                                                                          .03000
'FE'26. 055.9 07.110 00.707 0332 08.64 1.0000 0.320 01.937 01.757 17.600 095.800
    2.72 01.743 011.75 2.73 17.2   10.0   17.2   7.0     17.525
                                                                          .03250
'TI'22. 047.9 04.970 00.450 0270 09.45 1.0000 0.224 02.748 02.514 27.420 062.100
    2.73 02.497 007.00 2.73                                          27.3
                                                                          .02750
' O' 8. 016.0 00.532 00.000 0127 14.08 1.0000 0.004 23.700 00.000 50.000 003.800
    2.82 23.320
                                                                          .01000
 BOYD'S PROBLEM
0.          0.          0.          0.          0.          0.          0.          0.
0.1         .0334
 STANDARD #1.....PURE DIOPSIDE
   4  CA   MG   SI    O
18.51       11.23       25.93       44.33
 STANDARD #2.....ENAL 5
   4  MG   AL   SI    O
23.02       2.65        26.57       47.76
 STANDARD #3.....DI 65 JD 35
   6  CA   MG   SI   NA   AL    O
12.03        7.30        26.59       3.98        4.67        45.16
 STANDARD #4.....PYROPE GLASS
   5  MN   MG   AL   SI    O
4.19        16.29       12.05       20.95       46.52
 STANDARD #5.....CR IN MD 75 GLASS
   5  CA   MG   CR   SI    O
13.62       14.20       1.31        25.93       44.94
 STANDARD #6.....P-140 FOSTERITE
   4  MG   FE   SI    O
31.04       5.66        19.27       44.03
 BACKGROUND FOR AL
 BACKGROUND FOR FE
 BACKGROUND FOR CR
000010 0010000 0010000 0010000 211100
000010 0006240 0011170 0009690 111000
000010 0010000 0010000 0010000 212100
000010 0010000 0000000 0000000 221200
000010 0000000 0010000 0000000 221300
000010 0000000 0000000 0010000 221400
000010 0004350 0002210 0000215 121000
000010 0010000 0000000 0000000 222200
000010 0000000 0010000 0000000 222300
000010 0000000 0000000 0010000 222400
000010 0000010 0000000 0000000 322100
000010 0010000 0000000 0000000 231500
000010 0000000 0010000 0000000 231600
000010 0004500 0004550 0000000 131000
000010 0010000 0000000 0000000 232500
000010 0000000 0010000 0000000 232600
000010 0000010 0000000 0000000 332300
000010 0000000 0000010 0000000 3322001
```

Figure 11–Input Data – Sample Problem 1 – Intensity Data File

PARAMETERS USED

ELEMENT	CA	MG	SI	AL	NA	MN	CR	FE	TI	O
ATOM.NO	20.0000	12.0000	14.0000	13.0000	11.0000	25.0000	24.0000	26.0000	22.0000	8.0000
ATOM.WT	40.1000	24.3000	28.1000	27.0000	23.0000	54.9000	52.0000	55.9000	47.9000	16.0000
K ALPHA	3.3590	9.8890	7.1260	8.3370	11.9100	2.1030	2.2910	1.9370	2.7480	23.7000
K BETA	3.0900	9.5590	6.7680	7.9810	11.6170	1.9100	2.0850	1.7570	2.5140	0.0
K EDGE	3.0700	9.5120	6.7380	7.9510	11.4800	1.8960	2.0700	1.7430	2.4970	23.3200
L ALPHA	36.3300	50.0000	50.0000	50.0000	50.0000	19.5000	21.6400	17.6000	27.4200	50.0000
L3 EDGE	35.5000	250.7000	123.0000	170.4000	0.0	19.1000	20.7000	17.5250	27.3000	0.0
CK	48.4000	11.7500	18.5000	14.8700	9.0500	86.7000	79.0000	95.8000	62.1000	3.9000
NK	2.7400	2.7900	2.7700	2.7800	2.7900	2.7200	2.7300	2.7200	2.7300	2.8200
CKL	5.1900	3.8900	1.5400	1.1800	0.6200	10.4500	9.1800	11.7500	7.0000	0.0
NKL	2.7300	2.7300	2.7300	2.7300	2.7300	2.7300	2.7300	2.7300	2.7300	0.0
L1	0.0	0.0	0.0	0.0	0.0	0.0	16.7000	17.2000	0.0	0.0
CL1	0.0	0.0	0.0	0.0	0.0	8.8500	7.8000	10.0000	0.0	0.0
L2	0.0	0.0	0.0	0.0	0.0	0.0	17.9000	17.2000	0.0	0.0
CL2	0.0	0.0	0.0	0.0	0.0	5.9000	4.8000	7.0000	0.0	0.0
CLM	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
M1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CM1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
M2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CM2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
M3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CM3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
M4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
M5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CMN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VC(Z,K)	4.0410	1.8300	1.8400	1.5600	1.0700	6.5400	5.9900	7.1100	4.9700	0.5320
VC(Z,L)	0.3490	0.0490	0.1000	0.0750	0.0	0.0	0.5980	0.7070	0.4500	0.0
J1(Z)	239	133	154	142	126	316	301	332	270	127
RK(Z)	9.9200	12.3500	11.6400	11.9900	12.7400	8.8300	9.0300	8.6400	9.4500	14.0800
DXY(Z)	1.0000	1.0000	0.5000	0.6667	2.0000	1.0000	1.0000	1.0000	1.0000	1.0000
OMEGA-K	0.1810	0.0300	0.0560	0.0420	0.0200	0.2900	0.2680	0.3200	0.2240	0.0040
OMEGA-L	0.0250	0.0150	0.0175	0.0162	0.0137	0.0312	0.0300	0.0325	0.0275	0.0100
LINE	K	K	K	K	K	K	K	K	K	K
SPEC.NO	1	2	3	1	2	3	1	2		

VO	20.0000
THETA	52.5200
TAU	0.15000E-05 0.30000E-05 0.15000E-05
N	8
NM	6
NBGS	3
MODE	1
NPROB	1

Figure 12–Output Data – Sample Problem 1

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) – KALPHA RADIATION

	CA	MG	SI	AL	NA	MN	CR	FE	TI	O
CA	139.4	2656.7	1086.0	1667.0	4413.7	371.0	469.2	296.2	772.2	28882.3
MG	385.3	463.6	2815.0	4361.7	770.2	93.5	118.7	74.3	197.2	5040.2
SI	530.6	802.2	327.9	503.4	1332.8	145.0	183.8	115.5	304.3	8721.3
AL	431.7	614.7	3493.2	385.7	1021.2	117.4	149.0	93.4	247.0	6682.6
NA	265.9	5409.1	2168.1	3359.4	536.6	72.0	91.4	57.2	151.9	3511.2
MN	285.5	5443.5	2225.3	3415.6	9043.9	79.5	100.5	63.5	165.1	59180.5
CR	250.8	4782.0	1954.8	3000.5	7944.7	69.9	88.2	474.2	145.0	0.0
FE	321.1	6120.7	2502.1	3840.5	10168.9	89.4	113.0	71.4	185.6	0.0
TI	191.3	3646.4	1490.6	2288.0	6058.1	472.5	597.0	377.5	110.6	39642.4
O	115.8	2432.8	965.6	1503.2	4110.1	30.9	39.4	24.5	65.7	0.0

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) – LALPHA RADIATION

	CA	MG	SI	AL	NA	MN	CR	FE	TI	O
CA	99703.0	0.0	0.0	0.0	0.0	16957.6	22533.1	12817.9	43002.5	0.0
MG	16177.6	0.0	0.0	0.0	0.0	2959.3	3932.2	2236.9	7504.3	0.0
SI	27992.7	0.0	0.0	0.0	0.0	5120.5	6804.1	3870.5	12985.1	0.0
AL	21448.9	0.0	0.0	0.0	0.0	3923.5	5213.5	2965.7	9949.6	0.0
NA	11469.8	0.0	0.0	0.0	0.0	2061.5	2739.3	1558.3	5227.7	0.0
MN	*******	0.0	0.0	0.0	0.0	34746.4	46170.8	26264.2	88112.9	0.0
CR	0.0	0.0	0.0	0.0	0.0	15960.1	0.0	19603.9	0.0	0.0
FE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TI	*******	0.0	0.0	0.0	0.0	23275.1	30927.8	17593.2	59023.6	0.0
O	0.0	0.0	0.0	0.0	0.0	16507.5	22141.5	12363.1	0.0	0.0

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) – KBETA RADIATION

	CA	MG	SI	AL	NA	MN	CR	FE	TI	O
CA	111.0	2420.9	943.5	1479.7	4123.6	285.0	362.4	226.7	605.1	0.0
MG	273.5	422.5	2437.9	3861.7	719.6	71.5	91.3	56.6	153.8	0.0
SI	421.1	731.0	284.0	446.8	1245.2	111.1	141.6	88.1	237.8	0.0
AL	342.3	560.1	3026.8	342.4	954.1	89.9	114.7	71.2	192.9	0.0
NA	210.7	4918.9	1877.7	2974.3	501.3	55.0	70.3	43.6	118.5	0.0
MN	227.4	4960.4	1933.2	3032.0	8449.3	61.1	77.7	401.6	129.5	0.0
CR	199.7	4357.6	1698.2	2663.5	7422.5	456.4	68.2	363.3	113.7	0.0
FE	255.6	5577.5	2173.7	3409.2	9500.4	68.7	87.3	54.7	145.6	0.0
TI	152.3	3322.8	1295.1	2031.0	5659.8	363.3	461.6	289.3	85.7	0.0
O	91.5	2210.3	835.0	1329.2	3831.3	23.6	30.2	18.6	51.1	0.0

Figure 12–Output Data – Sample Problem 1 (Continued)

ELEMENT CHART – WEIGHT PERCENT

DATA PT	NO ITER	CA	MG	SI	AL	NA	MN	CR	FE	TI	O	SUM
*	*	11.544	12.548	25.125	1.150	0.878	0.050	0.588	2.568	0.100	43.724	98.375
*	*	11.535	12.742	25.924	1.166	0.917	0.091	0.580	2.585	0.100	44.755	100.256
*	2	11.561	12.849	26.037	1.172	0.926	0.091	0.581	2.587	0.100	44.574	100.772
*	3	11.567	12.845	26.084	1.175	0.928	0.091	0.581	2.587	0.100	45.048	101.927

FINAL CORRECTIONS: CA & FE GIVEN AS EXAMPLES

CA

MN-K ALPHA FLUORESCEN CA-K . KF= 0.552886E-04 CC MN)= 0.505566E-03
MN-K BETA FLUORESCEN CA-K . KF= 0.437568E-05 CC MN)= 0.588566E-03
CR-K ALPHA FLUORESCEN CA-K . KF= 0.479191E-02 CC CR)= 0.586077E-02
CR-K BETA FLUORESCEN CA-K . KF= 0.421832E-04 CC CR)= 0.586077E-02
FE-K ALPHA FLUORESCEN CA-K . KF= 0.121228E-02 CC FE)= 0.258272E-01
FE-K BETA FLUORESCEN CA-K . KF= 0.104488E-03 CC FE)= 0.258272E-01
TI-K ALPHA FLUORESCEN CA-K . KF= 0.347552E-03 CC TI)= 0.193CCE-02
TI-K BETA FLUORESCEN CA-K . KF= 0.225482E-04 CC TI)= 0.200116E-02
TOTAL FLUORESCENCE CORRECTION FOR CA= 0.100231E 01

FLUORESCENCE CORRECTION (FLU)
FLU = 1.003205
FLN = 1.000000
FLD = 1.000000

ABSORPTION CORRECTION (ABS)
APS = 0.958486
APN = 0.956633
APD = 0.955169

ATOMIC NUMBER CORRECTION (ANC)
ANC= 1.00176
ATN= 0.942041
ATD= 0.941988
SPU= 0.975577E 00
SPU= 0.222485E 01
PPS= 0.926018E 00
SPS= 0.220654E 01

FE

NO ELEMENT FLUORESCED FE . . . KF (TOTAL) = 1.0

FLUORESCENCE CORRECTION (FLU)
FLU = 1.000000
FLN = 1.000000
FLD = 1.000000

ABSORPTION CORRECTION (ABS)
APS = 0.958474
APN = 0.956479
APD = 0.955231

ATOMIC NUMBER CORRECTION (ANC)
ANC= 1.00185
ATN= 0.942041
ATD= 0.941988
SPU= 0.975577E 00
SPU= 0.222485E 01
PPS= 0.926018E 00
SPS= 0.220654E 01

Figure 12–Output Data – Sample Problem 1 (Continued)

```
 STANDARD # 1
THERE ARE  4 ELEMENTS IN THIS SAMPLE :     CA       MG       SI        O
WEIGHT PERCENTAGES /100 FOR THE ELEMENTS: 0.1881  0.1137  0.2593  0.4389

ATOMIC NUMBER CORRECTION=  *.*******E-**

ABSORPTION CORRECTION FOR CA.....CHI=  *.*******E-**        F(CHI)=  0.961688E 00
NO ELEMENT FLOURESCED CA...KF(TOTAL)=  *.*

ABSORPTION CORRECTION FOR MG.....CHI=   .*******E 04        F(CHI)=  0.883333E 00
CA-K ALPHA  FLOURESCED MG-K .     KF=  *.*******E-**        C( CA )=  0.189108E 00
CA-K BETA   FLOURESCED MG-K .     KF=  *.*******E-**        C( CA )=  0.189108E 00
SI-K ALPHA  FLOURESCED MG-K .     KF=   .********E-**       C( SI )=  0.188030E 00
SI-K BETA   FLOURESCED MG-K .     KF=  *.*******E-**        C( SI )=  0.188030E 00
TOTAL FLOURESCENCE CORRECTION FOR MG=  *.*******E 01

ABSORPTION CORRECTION FOR SI.....CHI=  *.*******E 04        F(CHI)=  0.672814E 00
CA-K ALPHA  FLOURESCED SI-K .     KF=  *.*******E-**        C( CA )=  0.188108E 00
CA-K BETA   FLOURESCED SI-K .     KF=  *.*******E-**        C( CA )=  0.188108E 00
TOTAL FLOURESCENCE CORRECTION FOR SI=  *.*******E 01


 STANDARD # 2
THERE ARE  4 ELEMENTS IN THIS SAMPLE :     MG       AL       SI        O
WEIGHT PERCENTAGES /100 FOR THE ELEMENTS: *.*******  *.*******  *.*******  *.*******

ATOMIC NUMBER CORRECTION=  *.*******E-**

ABSORPTION CORRECTION FOR AL.....CHI=  *.*******E 04        F(CHI)=  *.*******E 00
SI-K ALPHA  FLOURESCED AL-K .     KF=  *.*******E-**        C( SI )=  *.*******E 00
SI-K BETA   FLOURESCED AL-K .     KF=  *.*******E-**        C( SI )=  *.*******E 00
TOTAL FLOURESCENCE CORRECTION FOR AL=  *.*******E 01


 STANDARD # 3
THERE ARE  6 ELEMENTS IN THIS SAMPLE :     CA       MG       SI       NA       AL        O
WEIGHT PERCENTAGES /100 FOR THE ELEMENTS: *.*******  *.*******  *.*******  *.*******  *.*******  *.*******

ATOMIC NUMBER CORRECTION=  *.*******E-**

ABSORPTION CORRECTION FOR NA.....CHI=  *.*******E 04        F(CHI)=  0.956488E 00
CA-K ALPHA  FLOURESCED NA-K .     KF=  *.*******E-**        C( CA )=  0.120308E 00
CA-K BETA   FLOURESCED NA-K .     KF=  *.*******E-**        C( CA )=  0.120308E 00
MG-K ALPHA  FLOURESCED NA-K .     KF=  *.*******E-**        C( MG )=  *.*******E-**
MG-K BETA   FLOURESCED NA-K .     KF=  *.*******E-**        C( MG )=  *.*******E-**
SI-K ALPHA  FLOURESCED NA-K .     KF=  *.*******E-**        C( SI )=  0.266908E 00
SI-K BETA   FLOURESCED NA-K .     KF=  *.*******E-**        C( SI )=  0.266908E 00
AL-K ALPHA  FLOURESCED NA-K .     KF=  *.*******E-**        C( AL )=  0.467008E-01
AL-K BETA   FLOURESCED NA-K .     KF=  *.*******E-**        C( AL )=  0.467008E-01
TOTAL FLOURESCENCE CORRECTION FOR NA=  *.*******E 01


 STANDARD # 4
THERE ARE  5 ELEMENTS IN THIS SAMPLE :     NA       MG       AL       SI        O
WEIGHT PERCENTAGES /100 FOR THE ELEMENTS: 0.1415  *.1620  0.1265  0.2695  0.4802

ATOMIC NUMBER CORRECTION=  *.*******E-**

ABSORPTION CORRECTION FOR NA.....CHI=  *.*******E 04        F(CHI)=  0.970599E 00
NO ELEMENT FLOURESCED NA...KF(TOTAL)=  1.0


 STANDARD # 5
THERE ARE  5 ELEMENTS IN THIS SAMPLE :     CA       MG       CR       SI        O
WEIGHT PERCENTAGES /100 FOR THE ELEMENTS: 0.1363  0.1429  0.0131  0.2593  0.4484

ATOMIC NUMBER CORRECTION=  *.*******E-**

ABSORPTION CORRECTION FOR CR.....CHI=  *.*******E 03        F(CHI)=  0.944654E 00
NO ELEMENT FLOURESCED CR...KF(TOTAL)=  1.0


 STANDARD # 6
THERE ARE  4 ELEMENTS IN THIS SAMPLE :     MG       FE       SI        O
WEIGHT PERCENTAGES /100 FOR THE ELEMENTS: 0.1114  *.*****E  0.1927  0.4483

ATOMIC NUMBER CORRECTION=  *.*******E-**

ABSORPTION CORRECTION FOR FE.....CHI=  *.*******E 03        F(CHI)=  0.977715E 00
NO ELEMENT FLOURESCED FE...KF(TOTAL)=  1.0
```

Figure 12–Output Data – Sample Problem 1 (Continued)

DATA FILE

```
 &DATA THETA=52.5,TAU=3*0.,V0=20.0,M=2,NRGS=2,N=2,NFU=2,
 NM=2,BSTD(1)=1,BSTD(2)=2,STD(1,1)=1,STD(2,1)=2,NSTCOM=1,
 MODE=1,NPROB=1,LINE(1)='K',LINE(2)='L',ISPEC(1)=1,ISPEC(2)=2,
 &END
```

ELEMENT FILE

```
'TI'22. 047.9 04.970 00.450 0270 09.45 1.0000 0.224 02.748 02.514 27.420 062.100
   2.73 02.497 007.00 2.73                                    27.3
                                                                .02750
'NB'41. 092.9 30.000 02.370 0553 00.00 1.0000 0.796 00.746        05.724
                 045.50 2.73 04.581 038.90 05.026 027.90 05.223 008.30
                                                                .05600
```

COMPLETION FILE

```
UNKNOWN
0.
 STANDARD-PURE TI
   1  TI
100.
 STANDARD-PURE NB
   1  NB
100.
      BACKGROUND FOR TI
      BACKGROUND FOR NB
```

INTENSITY DATA FILE

```
000001 0C2510C 0000000 0000000 2111000
000001 0000000 0010100 0000000 2112000
000001 0000160 0000000 0000000 3111000
000001 0000140 0000000 0000000 3111000
000001 0000000 0000135 0000000 3112000
000001 0000000 0000125 0000000 3112000
000001 0008300 0006330 0000000 1111000
000001 0025100 0000000 0000000 2121000
000001 0000000 0010100 0000000 2122001
```

Input Data — Sample Problem 2

PARAMETERS USED

ELEMENT	TI	NB
ATOM.NO	22.0000	41.0000
ATOM.WT	47.9000	92.9000
K ALPHA	2.7490	0.7450
K BETA	2.5140	0.0
K EDGE	2.4970	0.0
L ALPHA	27.4200	5.7240
L3 EDGE	27.3000	5.2230
CK	62.1000	0.0
NK	2.7300	0.0
CKL	7.0000	45.5000
NKL	2.7300	2.7300
L1	0.0	4.5810
CL1	0.0	38.9000
L2	0.0	5.0260
CL2	0.0	37.9000
CLM	0.0	8.3900
M1	0.0	0.0
CM1	0.0	0.0
M2	0.0	0.0
CM2	0.0	0.0
M3	0.0	0.0
CM3	0.0	0.0
M4	0.0	0.0
M5	0.0	0.0
CMN	0.0	0.0
N1	0.0	1.0
VC(Z,K)	4.5700	0.0
VC(Z,L)	0.4500	3.3700
J1(Z)	270	553
RK(Z)	9.4500	1.0
DXY(Z)	1.0000	1.0000
OMEGA-K	0.2240	0.7960
OMEGA-L	0.0275	0.0560
LINE	K	L
SPEC.NO	1	2
V0	20.0000	
THETA	52.5000	
TAU	0.0	0.0 0.0
N	2	
NM	2	
NRGS	2	
MODE	1	
NPROB	2	

MASS ABSORPTION COEFFICIENTS

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) -- KALPHA RADIATION

	TI	NB
TI	111.6	27.9
NB	718.7	20.4

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) -- LALPHA RADIATION

	TI	NB
TI	59023.0	819.6
NB	45907.7	783.0

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) -- KBETA RADIATION

	TI	NB
TI	86.7	0.0
NB	563.6	0.0

Figure 14–Output Data – Sample Problem 2

```
IN STANDARD COMBINATION #     1   TI USES STANDARD #   1

IN STANDARD COMBINATION #     1   NB USES STANDARD #   2
```

ELEMENT CHART – WEIGHT PERCENT

DATA PT	NO ITER	TI	NB	SUM
1	0	32.665	62.187	94.852
2	1	34.491	64.646	99.137
3	2	34.712	65.332	100.044
4	3	34.762	65.462	100.224

FINAL CORRECTIONS

```
NO ELEMENT FLOURESCED TI...KF(TOTAL)=   0.0
```

FLUORESCENCE CORRECTION (FLU)

```
FLU =    1.00000
FLN =    1.00000
FLD =    1.00000
```

ABSORPTION CORRECTION (ABS)

```
ABS =    0.87303
ABN =    0.83675
ABD =    0.95845
```

ATOMIC NUMBER CORRECTION (ANC)

```
ANC=     1.07604
ATN=     0.51920
ATD=     0.48251
RBU=     0.80462E 00
SBU=     0.15497E 01
RBS=     0.98366E 00
SBS=     0.18714E 01
```

```
TI-K ALPHA  FLOURESCED NB-L .      KF=   0.36801E-02        C( TI )=   0.34762E 00
TI-K BETA   FLOURESCED NB-L .      KF=   0.32807E-03        C( TI )=   0.34762E 00
TOTAL FLOURESCENCE CORRECTION FOR NB=   0.10040E 01
```

FLUORESCENCE CORRECTION (FLU)

```
FLU =    1.00401
FLN =    1.00401
FLD =    1.00000
```

ABSORPTION CORRECTION (ABS)

```
ABS =    0.99238
ABN =    0.75041
ABD =    0.75617
```

ATOMIC NUMBER CORRECTION (ANC)

```
ANC=     0.95305
ATN=     0.51920
ATD=     0.54476
RBU=     0.80462E 00
SBU=     0.15497E 01
RBS=     0.75989E 00
SBS=     0.13949E 01
```

Figure 14–Output Data – Sample Problem 2 (continued)

DATA FILE

```
&DATA THETA=52.5,TAU=.15E-5,.30E-5,.15E-5,MODE=2,V0=20.0,
STD(1,1)=3,STD(2,1)=4,STD(3,1)=2,STD(4,1)=1,
N=4,NEU=4,M=4,
LINE(1)='K',LINE(2)='K',LINE(3)='L',LINE(4)='K',
ISPEC=1,2,3,1,5*0,NPROB=3,NSTCOM=1,NM=4,NRGS=0,
&END
```

ELEMENT FILE

```
'AL'13. 027.0 01.560 00.075 0142 11.99 0.6667 0.042 08.337 07.981 50.000 014.870
   2.78 07.951 001.18 2.73                                        170.4
                                                                  .01625
'MG'12. 024.3 01.300 00.045 0133 12.35 1.0000 0.030 09.889 09.558 50.000 011.750
   2.79 09.512 000.89 2.73                                        250.7
                                                                  .01500
'AU'79. 197.2 00.000 11.900 1071 00.00 1.0000 1.784                    01.276
               272.00 2.59 00.863 232.00 00.903 167.00 01.040 067.64 03.620
   058.3 03.939 48.3 04.522 41.8 05.415 05.629 22.50               .365
'CU'29. 063.5 08.980 00.933 0377 08.12 1.0000 0.410 01.542 01.392 13.400 126.800
   2.71 01.380 016.45 2.73 11.270 014.06 13.01  10.1   13.29
                                                                  .03625
```

COMPOSITION FILE

```
MODE 2 PROBLEM
10.        50.        40.        0.1
 STANDARD #1.....PURE COPPER
   1  CU
100.
 STANDARD #2.....PURE GOLD
   1  AU
100.
 STANDARD #3.....PURE ALUMINUM
   1  AL
100.
 STANDARD #4.....PURE MAGNESIUM
   1  MG
100.
```

Figure 15–Input Data – Sample Problem 3

ELEMENT	AL	MG	AU	CU
ATOM.NO	13.0000	12.0000	79.0000	29.0000
ATOM.WT	27.0000	24.3000	197.2000	63.5000
K ALPHA	8.3370	9.8890	0.0	1.5420
K BETA	7.9810	9.5580	0.0	1.3920
K EDGE	7.9510	9.5120	0.0	1.3800
L ALPHA	50.0000	50.0000	1.2760	13.4000
L3 EDGE	170.4000	250.7000	1.0400	13.2900
CK	14.8700	11.7500	0.0	126.8000
NK	2.7800	2.7900	0.0	2.7100
CKL	1.1800	0.8900	272.0000	16.4500
NKL	2.7300	2.7300	2.5900	2.7300
L1	0.0	0.0	0.8630	11.2700
CL1	0.0	0.0	232.0000	14.0600
L2	0.0	0.0	0.9030	13.0100
CL2	0.0	0.0	167.0000	10.1000
CLM	0.0	0.0	67.6400	0.0
M1	0.0	0.0	3.6200	0.0
CM1	0.0	0.0	58.3000	0.0
M2	0.0	0.0	3.9390	0.0
CM2	0.0	0.0	48.3000	0.0
M3	0.0	0.0	4.5220	0.0
CM3	0.0	0.0	41.8000	0.0
M4	0.0	0.0	5.4150	0.0
M5	0.0	0.0	5.6250	0.0
CMN	0.0	0.0	22.5000	0.0
NI	0.0	0.0	0.0	0.0
VC(Z,K)	1.5600	1.3000	0.0	8.9800
VC(Z,L)	0.0750	0.0490	11.9000	0.9330
J1(Z)	182	133	1071	377
RK(Z)	11.9500	12.3500	0.0	8.1200
OXY(Z)	0.6667	1.0000	1.0000	1.0000
OMEGA-K	0.0420	0.0300	1.7840	0.4100
OMEGA-L	0.0162	0.0150	0.3650	0.0362
LINE	K	K	L	K
SPEC.NO	1	2	3	1
V0	20.0000			
THETA	52.5000			
TAU	0.15000E-05	0.30000E-05	0.15000E-05	
N	4			
NM	4			
NBGS	0			
MODE	2			
NPROB	3			

MASS ABSORPTION COEFFICIENTS

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) -- KALPHA RADIATION

	AL	MG	AU	CU
AL	385.7	614.7	0.0	49.6
MG	4361.7	463.6	0.0	39.3
AU	16781.4	26157.7	0.0	208.6
CU	5376.8	8569.0	0.0	53.7

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) -- LALPHA RADIATION

	AL	MG	AU	CU
AL	0.0	0.0	29.3	1408.9
MG	0.0	0.0	23.2	1062.6
AU	*******	*******	127.5	57633.6
CU	0.0	0.0	245.5	0.0

MASS ABSORPTION COEFFICIENTS (EMITTER AT TOP) -- KBETA RADIATION

	AL	MG	AU	CU
AL	342.4	561.1	0.0	37.3
MG	3861.7	422.5	0.0	29.6
AU	14981.4	23941.8	0.0	159.8
CU	4772.9	7606.5	0.0	40.6

Figure 16–Output Data – Sample Problem 3

```
AU-L ALPHA  FLOURESCED AL-K .       KF=  0.15917E-04          C( AU )=  0.40000E 00
CU-K ALPHA  FLOURESCED AL-K .       KF=  0.13237E-06          C( CU )=  0.10000E-02
CU-K BETA   FLOURESCED AL-K .       KF=  0.10667E-07          C( CU )=  0.10000E-02
TOTAL FLOURESCENCE CORRECTION FOR AL=  0.10000E 01

   FLUORESCENCE CORRECTION (FLU): AL
      FLU =    1.00002
      FLN =    1.00002
      FLD =    1.00000

   ABSORPTION CORRECTION (ABS): AL
      ABS =    0.21365
      ABN =    0.161 8
      ABD =    0.84080

   ATOMIC NUMBER CORRECTION (ANC): AL
      ANC=     1.[illegible]
      ATN=     0.[illegible]
      ATD=     0.[illegible]
      RBU=     0.[illegible]
      SBU=     0.[illegible]
      RBS=     0.[illegible]
      SBS=     0.[illegible]


AL-K ALPHA  FLOURESCED MG-K .       KF=  0.[illegible]        C( AL )=  0.[illegible]
AL-K BETA   FLOURESCED MG-K .       KF=  0.[illegible]        C( AL )=  0.[illegible]
AU-L ALPHA  FLOURESCED MG-K .       KF=  0.[illegible]        C( AU )=  0.[illegible]
CU-K ALPHA  FLOURESCED MG-K .       KF=  0.[illegible]        C( CU )=  0.[illegible]
CU-K BETA   FLOURESCED MG-K .       KF=  0.[illegible]        C( CU )=  0.[illegible]
TOTAL FLOURESCENCE CORRECTION FOR MG=  0.[illegible]

   FLUORESCENCE CORRECTION (FLU): MG
      FLU =    1.[illegible]
      FLN =    1.[illegible]
      FLD =    1.[illegible]

   ABSORPTION CORRECTION (ABS): MG
      ABS =    0.18207
      ABN =    0.[illegible]
      ABD =    0.87247

   ATOMIC NUMBER CORRECTION (ANC): MG
      ANC=     1.17291
      ATN=     0.48444
      ATD=     0.41306
      RBU=     0.85904E 00
      SBU=     0.17581E 01
      RBS=     0.99577E 00
      SBS=     0.32407E 01

NO ELEMENT FLOURESCED AU...KF(TOTAL)=  1.0

   FLUORESCENCE CORRECTION (FLU): AU
      FLU =    1.00000
      FLN =    1.00000
      FLD =    1.00000

   ABSORPTION CORRECTION (ABS): AU
      ABS =    1.01377
      ABN =    0.96435
      ABD =    0.97098

   ATOMIC NUMBER CORRECTION (ANC): AU
      ANC=     0.70547
      ATN=     0.48444
      ATD=     0.68670
      RBU=     0.98984E 00
      SBU=     0.17581E 01
      RBS=     0.78228E 00
      SBS=     0.11428E 01


AU-L ALPHA  FLOURESCED CU-K .       KF=  0.73051E-01          C( AU )=  0.40000E 00
TOTAL FLOURESCENCE CORRECTION FOR CU=  0.10731E 01

   FLUORESCENCE CORRECTION (FLU): CU
      FLU =    1.07305
      FLN =    1.07305
      FLD =    1.00000

   ABSORPTION CORRECTION (ABS): CU
      ABS =    0.99395
      ABN =    0.98774
      ABD =    0.99382

   ATOMIC NUMBER CORRECTION (ANC): CU
      ANC=     0.68370
      ATN=     0.48444
      ATD=     0.70792
      RBU=     0.88564E 00
      SBU=     0.17581E 01
      RBS=     0.89804E 00
      SBS=     0.17760E 01


  MODE 2 PROBLEM:  INPUT-COMPOSITION RATIOS...OUTPUT-INTENSITY RATIOS
PROBLEM#     3
ELEMENT.....INTENSITY RATIO-SAMPLE TO STANDARD-ATN*ABN*FLN*C(U)/ATD*ABD*FLD*C(S)
   AL              0.24227E-01
   MG              0.10687E 00
   AU              0.29937E 00
   CU              0.10070E-02
```

Figure 16–Output Data – Sample Problem 3 (Continued)

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