A Rigorous Correction Procedure for Quantitative Electron Probe Microanalysis (COR 2)
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A Rigorous Correction Procedure for Quantitative Electron Probe Microanalysis (COR 2)

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A Rigorous Correction Procedure for Quantitative Electron Probe Microanalysis (COR 2)

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This publication describes a rigorous data reduction procedure for quantitative electron probe microanalysis, which avoids simplifications present in conventional schemes. In addition, the program contains a correction for fluorescence due to the continuum, and separate computation of the fluorescent effects of each exciting primary x-ray line. Constants characteristic of elements are stored in a permanent data file, and the constants and parameters needed for the calculation of mass absorption coefficients are contained in a sub-program. These provisions and decision-making sections in the development of the fluorescence corrections reduce the required input considerably.

Key words: Continuum fluorescence; data reduction; electron probe microanalysis; fluorescence correction; quantitative analysis.
1. Foreword

Quantitative electron probe analysis requires elaborate computer procedures for data reduction, unless standards of composition close to that of the specimen are available. For several years in the electron probe laboratory at NBS, a program called MULTI was used. The most recent version of this program - MULTI8 - was described in a recent Technical Note [1].

The program MULTI8 contains "corrections" for the primary generation ("atomic number correction") and absorption, and for fluorescence caused by characteristic lines (according to Reed [2]). There are, however, no provisions in MULTI8 for the treatment of the effects of fluorescence due to continuous radiation. These effects are usually not very severe; tests on known materials have shown that MULTI8 performs to our entire satisfaction in analytical practice. Nevertheless, there is need for a more rigorous and complete program which permits an estimation of the errors due to the neglect of the fluorescence caused by the continuum, and to other approximations used in MULTI8 and other simplified programs which are used in routine work.

The project to obtain such a rigorous procedure, incorporating all known refinements of the theory, was initiated when J. Hénoc, of the C.N.E.T., Issy-les-Moulineaux, France, spent one year in the electron probe laboratory of NBS as a guest worker in 1969. Dr. Hénoc has previously developed a method for the calculation of the fluorescence due to the continuum [3]. He agreed to develop, in consultation with us, a program which would satisfy our needs.

The scheme of formal integration previously used in reference [3] was replaced with a numerical integration with respect to the wavelength of the exciting radiation. This change was necessary for the use of the expressions for x-ray mass absorption coefficients previously developed by one of us [4]. It also became evident that it would be easier to write an entirely new program for data reduction than to
incorporate the continuum-fluorescence calculation into existing procedures. The need for locating all x-ray absorption edges in the specimen for the treatment of fluorescence from the continuum suggested that the program could also determine which fluorescence excitations due to characteristic lines should apply. The procedure of Reed [2] was abandoned in favor of a separate computation of the effects of each exciting characteristic line; the intensity of every exciting line was computed by a full generation calculation. The resulting program was called COR.

Although we did not originally conceive of COR as a tool for routine analysis, we find that it can be used advantageously for this purpose wherever batch processing with a reasonably large computer is acceptable. The fact that the program calculates all necessary mass absorption coefficients and makes appropriate decisions concerning the applicability of fluorescence calculations is a distinct advantage over MULTI8 and similar programs, since the data input is considerably simplified. The difference in the results obtained by COR and by MULTI8 is frequently insignificant, except where fluorescence by the continuum is unusually large.

After a period of testing and use, we have introduced some minor changes into the program, which are mainly additions that enable us to use the M-lines for analysis, and an alternative in the input and readout procedures. In order to distinguish the amended program from the original, we call the new version COR 2.

The new version was cast into its present form on the occasion of a second visit by Dr. Hénoc in November 1972. We will describe this program in detail. It is useful to recall, however, that the main purpose of this publication is not only the description of a computer program, but also the presentation of a data evaluation procedure which is not used elsewhere, to our knowledge, in any form except that of COR and COR 2.

K. Heinrich
2. Specifications and Theoretical Foundations for COR 2

COR 2 is written for batch processing in FORTRAN IV, and occupies about 50K words. At NBS, it is run on the UNIVAC 1108 computer*, and elsewhere, with minor adaptation, on computers such as the IBM 360 and GE 635.

The program permits the loading, in a single operation, of repeated measurements at one point on the sample, of measurements on several points (up to 100), and of several types of analyses or specimens (cases).

In its present form, COR 2 permits the presence of up to 15 chemical elements per point. The limits indicated here can be changed simply by altering the corresponding dimension statements.

The program can calculate either theoretical relative intensities for specimens of known composition - without need for iteration - or the composition of analyzed specimens. For the analysis of specimens of unknown composition, either relative x-ray intensities or uncorrected x-ray intensity measurements are acceptable.

The composition of analyzed specimens is expressed both in weight fractions and in atomic fractions (in the conventional output). Each element can be measured at a different operating voltage. The iteration proceeds until two successive sets of mass fractions differ, for all elements, by less than $10^{-5}$ (0.001%), or, if convergence is not reached, until completion of 20 iterations. In such case, a warning message would be printed. In practice, convergence is usually obtained in three to six iterations; lack of convergence has never been observed.

*The computers are identified in order to adequately specify the use of the program. In no case does such identification imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the equipment identified is necessarily the best available for the purpose.
The following options of COR 2 can be used by means of switches provided in the program.

1. One element can be determined by difference.
2. One element can be determined by stoichiometric relations (and another by difference, if desired). In such cases, the results are also printed in terms of binaries (e.g., as oxides), and the stoichiometric formula is printed. (See the section concerning output, p. 65)
3. The concentration of one or more elements can be assumed known, and be maintained constant throughout the analysis. (e.g., for the analysis of impurities in a stoichiometric compound or in an element.)
4. In any of these variants, the correction for fluorescence due to the continuum can be suppressed.
5. The standards for measured elements may either be elements or multi-element materials of known composition.
6. A special output particularly useful for diagnostic purposes is available. This output is the one used in the original version of COR (output 2 or extended output).

As in other schemes of data reduction for electron probe microanalysis, the basic process imbedded in COR 2 is the calculation of a theoretical relative x-ray intensity emitted from a target of known or postulated composition. We will call this part of the procedure the "theoretical calculation", although we recognize the presence of empirical adjustment in almost all steps. The designation as "theoretical" merely distinguishes a procedure which contains separate corrections for primary generation, absorption, and fluorescence, from other approaches which require, at the time of the analysis, several compound standards to generate an empirical calibration model. For the analysis of specimens of unknown composition, the "theoretical calculation" is coupled with an iteration procedure which, starting with a rough estimate of specimen composition, proceeds to establish the best estimate by a method of successive approximations.
The theoretical or semi-empirical foundations of the method which we have followed were described in the NBS Technical Note 521, reproduced at the end of the present publication (see Appendix 1). The comments referring to COR in TN 521 are equally valid for the present version, COR 2. By modifying the corresponding statements in the correction functions, variants in the correction models can be introduced. The pertinent literature references are found in the Appendix.

3. **Structure of the Program**

COR 2 consists of a main program (MAIN), and a series of subprograms linked to the main program as shown in Figure 1. The **input** consists of a series of option specifications, a permanent data file, and the experimental x-ray intensities or known concentrations. The purpose of the specifications is to select among the options available for the execution of the program, such as use of stoichiometric relations, calculation of an element by difference, use of known concentration of some components (e.g., in the analysis of impurities of an element or of a stoichiometric compound), corrections for background and dead-time, and calculation of theoretical x-ray intensities for a target of known composition.

There are two versions of the **output** which can be selected by another code in the input. The conventional output (output 1) has been developed for COR 2. The extended output (output 2), which was used in the original version of COR, is particularly useful for the diagnosis of programming errors or similar problems. References to output, unless specified otherwise, refer to output 1.

The **data file** which forms part of the input contains constants specific for particular elements present in the specimens. We have added elements to this data file, as required, and keep it stored on a magnetic drum. Other
Figure 1. Structure of COR 2.
systems may require different procedures. On page 114 the reader will find instructions for adding the constants for elements not present in our file to the data file.

The input data can either be mass fractions of a known target, or relative x-ray intensities, corrected for background and dead-time ("k-values"), or uncorrected x-ray intensities (counts), for line, background and standard. In the latter case, an input specification directs the main program to transfer the x-ray intensities to the subprogram AINP, which performs the corrections for deadtime and background. If repeated measurements were performed at the same specimen location, AINP also provides statistics of the uncorrected intensities. The corrected relative intensities are returned to the main program.

The principal functions of MAIN are to perform the theoretical calculations of the x-ray intensities corresponding to an estimated target composition, and to refine the estimated mass fractions by means of the previously mentioned iteration procedure. The theoretical calculations are based on the equation:

\[
k = \frac{I_p' f_p^* + \sum I_f^* f_f^*}{\sum I_p' f_p^* + \sum I_f^* f_f^*} + \frac{I_c' f_c^*}{\sum I_c' f_c^*}
\]

in which \( k \) is the background- and deadtime-corrected relative x-ray intensity, \( I_1' \) signifies x-ray intensities generated within the specimen, \( f \) denotes the absorption factors, the subscripts \( p, f, \) and \( c \) indicate, respectively, primary emission, fluorescent emission excited by characteristic lines, and fluorescent emission excited by the continuum. The superscripts \( * \) and \( s \) denote, respectively, the specimen and the standard. The summation sign in the characteristic fluorescence terms indicates the possibility of excitation of a line by more than one exciting
line. If there is more than one exciting line, the fluorescence due to each line is calculated separately. The use of equation (1) replaces that of multiplicative correction factors according to the ZAF procedure, which is impractical when the fluorescence due to the continuum is considered (see p. 80, Appendix 1).

In the computation of $k$, MAIN is assisted by several subprograms. COCA starts by selecting the constants relevant to the elements and lines from the data provided by the data file. With the aid of these constants, MAIN directs CALI to establish a sequence of procedures for calculating the parameters necessary for equation (1). In this process, CALI utilizes the following subprograms:

PRA, to determine the intensities of primary emission $I_p'$, (which are also used in the characteristic fluorescence correction),

FQI, to determine the primary absorption factors, $f_p$,

FCA, to determine the characteristic fluorescence contributions, $I_f'f_f$,

CO, to determine the fluorescent intensity due to the continuum, $I_c'f_c$.

These subprograms in turn use the following subprograms for the calculation of needed parameters and integrals:

RB, to determine the backscatter correction function,

EI, to calculate exponential integrals,

AC, to calculate x-ray mass attenuation coefficients,

F, to perform the numerical integrations for the continuum fluorescence correction, and

FT, to perform the same integrations, with omission of the x-ray absorption (this is required only to determine the absorption term $f_c$, and could be omitted if this term is of no interest).

CALI, assisted by these subprograms, assembles the numerator and the denominator of the fraction on the right
side of equation (1). These are sent to MAIN, which calculates the relative intensity $k$ for all elements which have been measured, and initiates a step of iteration by the method outlined in the Appendix. If the purpose of the calculation was to establish theoretical intensities for a known composition, or if the results of the theoretical calculations for all elements match the results of the previous iteration (with a tolerance of $10^{-5}$), then the calculation is terminated, and the results are printed in the OUTPUT procedure.

Besides making the pertinent decisions concerning the application of fluorescence correction, the program incorporates warning messages which are transmitted to the output if needed parameters (e.g., mass absorption coefficients) are not available or cannot be reliably calculated, or if the operating conditions were chosen improperly. These two features of the COR program render it less susceptible to mistakes by the operator.
4. Explanation of the Program

4.1 MAIN Program

4.11 Input of the Contents of the Permanent Data File

At this point, the complete permanent data file is loaded.

READ (5,30) NELM  Read first card which contains the number of elements of which the constants are tabulated

loop 350:

READ (5,40) Read a card which contains the constants that depend on the atomic number only:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>J</td>
<td>atomic number of element</td>
</tr>
<tr>
<td>KM(J)</td>
<td>number of x-ray absorption edges</td>
</tr>
<tr>
<td>A(J)</td>
<td>atomic weight</td>
</tr>
<tr>
<td>FCK12(J)</td>
<td>Coster Kronig coefficients, f12, f23, f13</td>
</tr>
<tr>
<td>FCK23(J)</td>
<td></td>
</tr>
<tr>
<td>FCK13(J)</td>
<td></td>
</tr>
<tr>
<td>CI(J)</td>
<td>multiplicative constant for the mass absorption coefficients [4]: C_K if J&lt;50, C_KL if J&gt;50</td>
</tr>
<tr>
<td>ANK(J)</td>
<td>exponent n_K, for the mass absorption coefficients</td>
</tr>
<tr>
<td>ANKL(J)</td>
<td>exponent n_KL, for the mass absorption coefficients ((\mu)) according to (\mu = C\lambda^n)</td>
</tr>
</tbody>
</table>

loop 350

READ (5,50) Read a card containing the constants which depend on the atomic level:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>WAV(K,J)</td>
<td>wavelength of absorption jump</td>
</tr>
<tr>
<td>R(K,J)</td>
<td>jump ratio</td>
</tr>
<tr>
<td>OME(K,J)</td>
<td>fluorescence yield</td>
</tr>
<tr>
<td>LM(K,J)</td>
<td>number of tabulated lines for this level</td>
</tr>
</tbody>
</table>

implied loop

READ (5,70) Read cards containing line wavelengths and relative intensities:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CL(L,K,J)</td>
<td>wavelength of line</td>
</tr>
<tr>
<td>ZL(L,K,J)</td>
<td>relative intensity of line</td>
</tr>
</tbody>
</table>

1 All the variables used in this program are defined in Appendix 2.
Note: The levels are indexed 1,2,3,4,... for K,L_I,L_{II},L_{III}...
If there is no information for a level, an empty card must be
inserted. Do not insert a blank card at the end of the table
of constants for an element; otherwise, difficulties will
appear in calculating the absorption coefficients.

4.1.2 Input Specific to the Particular Analysis, to the
Specimen and to the Standards

READ (5,30) NECM  Read a card containing the number
of cases. Two cases are considered different if
the elements contained in them differ, or if the
conditions of analysis (voltage, line, etc.) differ.
loop 1010, concerning the handling of one case.

The tally of the numbers of iterations, NIT, is set to
zero, since intermediate parameters which are independent
of concentration are only printed after the first iteration.

The switch KST*OP* is set equal to 1, to assure the
start of the calculation. If an absorption coefficient
cannot be calculated in subprogram AC(CL,J), this switch
goes to 0.

READ (5,60) Read first card with information on
the case:

<table>
<thead>
<tr>
<th>JJM</th>
<th>number of elements contained in the specimen</th>
</tr>
</thead>
<tbody>
<tr>
<td>JJAM</td>
<td>number of elements analyzed</td>
</tr>
<tr>
<td>ND</td>
<td>switch indicating the mode of ratio input:</td>
</tr>
<tr>
<td></td>
<td>if it is 0 or if the field is empty:</td>
</tr>
<tr>
<td></td>
<td>direct input of relative x-ray intensities (k-values)</td>
</tr>
<tr>
<td></td>
<td>if it is 1, k-values are obtained by the subroutine AINP</td>
</tr>
<tr>
<td>NPM</td>
<td>number of points in the case.</td>
</tr>
<tr>
<td>LOUT</td>
<td>switch for choosing the version of output</td>
</tr>
<tr>
<td>ICOF</td>
<td>switch for suppression of continuum</td>
</tr>
<tr>
<td></td>
<td>fluorescence correction.</td>
</tr>
</tbody>
</table>

FIRST is a logical variable to detect the first
card of a case: punch a T. If the execution
of the program is stopped because of any diffi-
culty, the program proceeds to the next case.

*Switch, in the context of this paper, is a variable which
determines the option to be followed from a group of options.
ignoring the rest of the cards which belong to
the discarded case.

WRITE (6,160) NEC  Print case number (NEC).

Loop 430, for an analyzed element, calculates the intensity
of the standard.

READ (5,80)  Read a card identifying the element:

NZ(JJA)   atomic number
EØ        operating voltage
KA(JJA)   index for excited level
LA(JJA)   index for analyzed line
COSEC(JJA) cosecant of the x-ray emergence angle
NV(JJA)   valence, punch only if stoichiometry
          is to be calculated
NEST      if a composite standard is used,
          NEST is the number of elements
          present, besides that which is
          measured
CON(JJA)  switch for entering known concen-
          trations

The value of each concentration is now put to 1, for
all real or hypothetical standards. Then, the intensities
emerging from the standards are calculated as follows.

A call is made to CØCA (JJA,JJA,JJA) to obtain the input
necessary to calculate fluorescence due to the continuum,
and to introduce it into the CØMMØN memory.

If execution of CØCA (JJA,JJA,JJA) has not caused an
error message to be printed, the execution continues.
Otherwise, control is transferred to the next case.

Note that the switch NCØ (JJA) is tested immediately
after each execution of the program CØCA.

A call is made to CALI (JJA,JJA,JJA,AIT...) to calculate
the total emerging intensity of the standard AI. Then
the switch KSTØP is tested. If it has turned to 0
(i.e. we have a meaningless mass absorption coefficient),
a message is printed and control is transferred to the
point of reading data for the next case.

READ (5,100)  When the standard for an element is
composite (NEST#0) then a card gives the mass fraction
of this element in the standard. As many cards as
there are additional elements in the standard, give
for each element:
The subprograms C0CA (JJA,JST,JJA) and CALI (JJA,JST, JJA, AIT...) produce the ratio \( \text{AIR} (\text{JJA}) = \frac{I_A}{I(A)} \); this value is 1 for a simple standard.

The specimen is now characterized as follows:

A series of IF statements switches NSW into one of five possible positions:

- If all elements are analyzed, NSW→1
- If there are two unanalyzed elements, NSW→4 (one element by stoichiometry, another by difference)
- If there is one unanalyzed element, and valences were listed, NSW→2 (one element by stoichiometry)
- If a concentration is listed for the unanalyzed element, NSW→5 (calculate k-value for known composition)
- If none of the preceding is true, NSW→3 (calculate one element by difference)

If NSW was not switched to 1, the following READ statement is used to set NSW to the proper value:

\[
\text{READ (5,110)}
\]

\[
\begin{align*}
\text{NZ(JJ)} & \quad \text{atomic number of unanalyzed element} \\
\text{NV(JJ)} & \quad \text{its valence (empty unless stoichiometry is calculated)} \\
\text{CD(1,JJ)} & \quad \text{its concentration (empty unless k-values are calculated)}
\end{align*}
\]

The decision to calculate k-values from known concentrations is signaled through the input of a "known" concentration value for one element (JJA1) in CD(1,JJ). This tells the program that the C(JJA) values entered for the elements other than JJA1 are concentrations rather than k-values, and the k-values of these elements are calculated. But, JJA1 is an "unanalyzed" element, and its k-value is not calculated. In order to obtain the
k-values for all elements of a specimen of known composition, one must run it in two cases, changing the order of input of the element between two cases since the last element being entered is always the "unanalyzed" element 

JJAl.

The subprogram COCA (1,JJM,JJM) is called to determine the constants for fluorescence, in iteration no. 0 only for the measured lines of elements to be analyzed.

(loop 500).

The value of ND (p.12) indicates if the experimental k-values are entered by cards or through subprogram AINP (CD,NPM,JJAM,SD).

READ (5,100) If the input is by cards, this card, and the following, give the mass fractions or k-values of all measured elements for all points to be calculated. If relative intensities are input for more than one point of the same specimen, the k-values are read on the next card or cards for all points after the first point.

AINP (CD,NPM,JJAM,SD) is called if ND = 1 (output from the electron probe; output on punched cards or magnetic tape)

4.1.3 Calculation of Concentrations for Each Point

loop 1000; the subscript denotes the point on the specimen.

loop 550

As a first approximation, C = k. The k-value for each measured element is stored in a permanent memory location. The sum of concentrations is calculated.

The position of switch NSW now leads to the following instructions:

NSW=1: All elements present must be analyzed. The number of each point and the concentration of the elements are printed: instruction 630

NSW=2: One element is determined by stoichiometry. Instructions 560 and 630

NSW=3: One element is determined by difference; instructions 580 and 630

NSW=4: One element by difference, and another by stoichiometry; instructions 590 and 630

NSW=5: Calculation of k-values; instructions 610 and 630.
loop 620

Input of concentration of elements which are not calculated.

loop 650: Normalization of concentrations for calculation of k-values.

after 650: Switch NSW2, which will cause the advance to next iteration, is positioned to 2.

660: If NSW2 is equal to 1, print results, and pass on to the next point.

670: If NSW2 = 2, initiate another iteration (max. no. of iterations: 20), and, in the extended output, print the number of the iteration.

loop 730

Calculate k-values for each analyzed element.
Print the main steps of calculation and k-values, in iteration 0 only, if extended output (output 2) is used.
Obtain next approximation by the hyperbolic equation.
Sum concentrations.
According to the position of switch NSW, command is now transferred to one of the following instructions:

790: NSW2 switches to 1. Test for convergence follows.
750: Calculate one element by stoichiometry.
740: Calculate one element by difference.
770: Calculate one element by difference, another by stoichiometry.

loop 810: normalization of concentrations, test for difference of concentrations found in two successive iterations (convergence test).

Normalization of concentrations for elements which were not measured.

Printing of results.

End of loop 1000
End of loop 1010

END
4.2 SUBROUTINE COCA (J0,JM,JJA)

Arguments:

J0 : label of first element considered in the case
JM : label of last element considered in the case
JJA: label of analyzed element in the case

4.2.1 This Subroutine Prepares the Fluorescence Calculations and Determines the Value of the Constants Needed

Limitations and warnings:

a) If operating voltage is high enough to excite higher levels corresponding to a different series, a warning is given.

b) If the operating voltage is above 30 kV, a message is given.

c) If the wavelength chosen passes beyond the N3 edge, or if the operating voltage is too low to excite the selected line, a message will be printed and the case will be aborted.

1) Fluorescence excited by the continuum

If the characteristic line of the measured element is produced by the excitation level corresponding to the edge of wavelength \( \lambda_o \), it can be excited by continuous radiation of a wavelength between the Douane-Hunt limit, \( \lambda_o \), and \( \lambda \). As one crosses an edge of any element present, the constants for calculating mass absorption coefficients change. One must consider all edges of all elements between \( \lambda_o \) and \( \lambda_q \). Any of the edges between these limits constitutes a sublimit for the integration to be performed; the corresponding element is registered, and all parameters referring to wavelengths above this edge are entered in memory.

If the element under consideration is the one we analyze, we also enter in memory a new efficiency factor, \((r_{i-1})/r_j\) and a new effective fluorescence yield, \(\omega_{eff}\).

2) Fluorescence excited by characteristic lines

For each element, except the analyzed element, the characteristic lines at each level are compared with \( \lambda_o \); if the shell emitting the analyzed line can be excited with a sufficient yield, the exciting line is
counted and the label of the corresponding element and the index of the series are stored.

All wavelengths previously stored in memory, with the associated parameters, are rearranged in increasing order, for the calculation of the fluorescence produced by the continuous spectrum, and to determine \((r_i - 1)/r_j\) and \(\omega_{\text{eff}}\) of the analyzed element for fluorescence by characteristic lines.

The output of the program consists of: number of sub-limits and associated parameters, number of lines which excite fluorescence, and associated parameters; error messages, in case the user has caused the switch \(\text{NC}0(JJA)\) to be changed.

4.2.2 Commentary on \(\text{C}0\text{CA}(J0,JM,JJA)\) (see Figure 2)

The following preliminary steps are performed in the first block of instructions:

The switch \(\text{NC}0(JJA)\) is set to 1. This switch will go to 0 if the calculation becomes impossible.

The tally of starting points for integrations is set to 1. The first point will be \(\lambda_0\).

The tally \(I3\) which counts the number of lines exciting fluorescent radiation, is set to zero.

The following constants related to the analyzed element, \(JJA\), are stored:

- \(NZA\) its atomic number
- \(WAA\) the wavelength associated with the operating voltage \((\lambda_0)\)
- \(KAA\) the subscript of the shell emitting the characteristic lines \((\lambda_{\text{char}})\)
- \(F_{12}\)
- \(F_{23}\)
- \(F_{13}\)

Loop 450:

The subscript of the loop \((JJ)\) is the tally in the sequence of the elements contained in the specimen.

Beginning at the starting point of interval \((WAA, WAV(KAA,NZA)), (\lambda_0, \lambda_{\text{char}})\) the program searches for cases of characteristic fluorescent excitation.

The collection of information for fluorescence from the continuum concerning the integration interval ends before the signal instruction 260.
COCA(J0, JM, JJA)

PARAM. ELEM. JJA

FOR ALL ELEMENTS

DO 450
JJ ← J0, JM
EXPO(JJ), CC(JJ)

FOR ALL EDGES

DO 440
K ← 1, KMJ
WAV(K, J), WAA

IF WAV(K, J) > WAV(KAA, NZA)
1 T

EXPO(JJ), CC(JJ)

260

WAVE(I), JJJ(I)

I2 = 1

RR(I), EX(I)

260

RR(I), EX(I)

260

JJ ≠ JJA

F

RRR(I), OMEG(I)

440 T

450

SORT

RETURN

FIND LINES EXCITING CHAR. FLUORESCENCE

DO 430
L ← 1, LMKJ

CL(L, K, J) > WAV(KAA, NZA)

F

CHARAC. FLUOR

430

440

Figure 2. Flowsheet of Subroutine COCA.
Tally 12: The tally for the number of discontinuities within the interval (WAA, WAV(KAA,NZA)) is set to zero.

The atomic number of element NZ(JJ) is renamed J, for the purpose of entering the permanent data file.

The number of absorption edges KM(J) stored in the permanent data file is renamed as a non-subscripted integer, KMJ.

The following instructions, until and including instruction 60, have the purpose to define the coefficients $C_i$ and $n_i$ for computing the absorption coefficient of the element JJ at the wavelength WAA ($\lambda_0$). These coefficients are called CC(JJ,JJA) and EXPO (JJ,JJA) for the element JJ of a specimen in which the element JJA is being determined.

Loop 440:

The subscript (K) is that of the absorption edge.

The positions of switches KR1, KR2, K1, are set, as a function of K.

The wavelength WAV (K,J) of the edge having the subscript K of the element of atomic number J, is compared with diverse wavelengths:

1. If the permanent data files have indicated that $\text{WAV} (K,J) \leq 10^{-6} \text{Å}$, the program is instructed that the corresponding level does not exist and proceeds to the next edge, K+1.

2. If $\text{WAV} (K,J) \leq \text{WAA}$ (i.e. the edge is at a wavelength shorter than $\lambda_0$), transfer is made, depending on the position of switch KR1, to one of the sets of instructions subscripted 80 to 570, to readjust CC(JJ,JJA) and EXPO (JJ,JJA).

A message is printed if one passes the edge $M_{IV}$. Switch NC0(JJA) is thrown if R(KMJ) is missing in the input or if K=12 (i.e., the analyzed line falls beyond the $N_{III}$ edge of any element).

3. If WAA < WAV(KMJ) < WAV(KAA,NZA), the tally 12, which counts the absorption edges of element J, is advanced one unit. The tally of the starting points for integration, I, is also advanced one unit. The edge, and the corresponding element, are stored in WAVE(I,JJA) and JJJ(I,JJA); the remaining memory locations are reset to 0.
If the edge WAV(K,J) is the first of the respective element to fall within the interval, control goes to one of the sets of instructions 190 to 570, depending on switch KR2. If not so, switch Kl leads to 150-570. In either case, the absorption edge jump and the exponent $n$, valid at the right of the edge, are calculated. The values are stored as RR(I,JJ) and EX(I,JJA).

Switch NCØ goes to 0 if one passes the edge $N_{III}$. If the $M_{IV}$ edge is crossed, a warning message is printed.

Following instruction 260, if the element is the one which is being measured, the switches KAS and KK determine a set of instructions for computing the efficiency ratio $(r_{i-1}/r_i)$, and the effective fluorescence yield $\omega_{eff}$. These are stored in RRR(I,JJA) and $\bar{\Omega}$MEG(I,JJA).

If the element being considered differs from that of the analyzed element, its strongest lines are compared to the edge WAV(KAA,NZA).

If excitation can occur, the tallies I and I3 increase by one; the wavelength and the subscripts for the element, shell, and line are stored in WAVE(I,JJA), JJJ(I,JJA), KB(I,JJA), LB(I,JJA).

4. If WAV(K,J) > WAV (KAA,NZA), the program passes to the end of loop 450 and goes on to next element.

When all elements have been scanned, WAA is stored in WAVE (1,JJA), and JJJ(1,JJA) = 0.

At this point, for each value of $I \leq I_M$, one has assembled the following table:

<table>
<thead>
<tr>
<th>number: IM-I3M</th>
<th>starting points (continuum fluorescence)</th>
<th>number: I3M line exciting the fluorescence of JJA</th>
</tr>
</thead>
<tbody>
<tr>
<td>WAVE(I,JJA)</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>RR(I,JJA)</td>
<td>X</td>
<td>(X)</td>
</tr>
<tr>
<td>JJJ(I,JJA)</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>RRR(I,JJA)</td>
<td>(X)</td>
<td>0</td>
</tr>
<tr>
<td>$\bar{\Omega}$MEG(I,JJA)</td>
<td>(X)</td>
<td>0</td>
</tr>
<tr>
<td>EX(I,JJA)</td>
<td>X</td>
<td>(X)</td>
</tr>
<tr>
<td>KB(I,JJA)</td>
<td>0</td>
<td>X</td>
</tr>
<tr>
<td>LB(I,JJA)</td>
<td>0</td>
<td>X</td>
</tr>
</tbody>
</table>

X Storage in memory.
(X) Storage not needed or empty.
The nested loops 470 and 480 arrange the set of wavelengths, together with the associated quantities, in increasing order. Then, a permutation of the indices I ensues.

The memory locations in the preceding table, for øMEG(I,JJA) and RRR(I,JJA) associated with characteristic lines are empty. In loop 500 one transmits stepwise these quantities so as to define the efficiency ratio and effective fluorescence yield for every characteristic line.

Output

After the preceding process, the computer performs a rearrangement such that the first wavelengths, in number IMA(JJA), are the sublimits for integration (for the continuum) and that those following, in number MF(JJA), are those of the characteristic lines capable of exciting the fluorescence of the analyzed element JJA.

The subprogram returns the following quantities:

WAVE(I,JJA)
JJJ(I,JJA)
RR(I,JJA) if 1 ≤ I ≤ IMA(JJA)
EX(I,JJA) (for continuum fluorescence)
RRR(I,JJA)
øMEG(I,JJA)

WAVE(I,JJA)
JJJ(I,JJA)
RRR(I,JJA) if IMA(JJA) + 1 ≤ I ≤ MF(JJA) + IMA(JJA) + 1
øMEG(I,JJA) (for characteristic fluorescence)
KB(I,JJA)
LB(I,JJA)

4.3 FUNCTION CØ(JØ,JM,JJA,FC,FQC)

This program calculates the intensity of fluorescence due to the continuum, by means of a numerical integration. CØ is separate from CØCA(JØ,JM,JJA) because it requires concentrations; therefore it is used in each iteration, while CØCA(JØ,JM,JJA) is used only once.
4.4 FUNCTIONS $F(X,J_0,J_M,J_{JA})$ and $FT(X)$

Function $F$ calculates the expression for continuum fluorescence to be numerically integrated in $C_0(J_0,J_M,J_{JA})$.

Function $FT(X)$ does the same calculation, with omission of the absorption terms for continuum fluorescence. The purpose of this calculation is the computation of the absorption correction factor for fluorescence from the continuum ($f_c$, FQC). If this information is not of interest, the calculation of $FT(X)$ can be omitted.

4.5 FUNCTION $AC(CL,J)$

Calculates the x-ray absorption coefficient of atomic number $J$ and wavelength $CL$; and acts upon the switch KST0P if an error is detected (i.e., if the coefficient cannot be calculated). The parameters given by Heinrich [7] are used.

4.6 FUNCTION $PRA(J_0,J_M,L_X,K_X,J_X,W_{AA})$

Calculates the intensity of primary emission of the line $L_X$, shell $K_X$, of the element of atomic number $J_X$, for a case containing the elements subscripted $J_0$ to $J_M$, where the Duane-Hunt limit associated with the energy of the electrons, $\lambda_o$, is $W_{AA}$.

4.7 FUNCTION $RB(U_0,Z)$

Calculates the backscatter correction $R$ of the element of atomic number $Z$ for the overvoltage $U_0$.

4.8 FUNCTION $FQI(J_0,J_M,L_X,K_X,J_X,W_{AA})$

Calculates the absorption correction $f$, commonly called $f(\chi)$, corresponding to the primary intensity $PRA$; the arguments have the same meaning as in $PRA$.

4.9 SUBROUTINE $FCA(J_0,J_M,L_{II},J_{JA},FCA_1,FCA_0)$

Calculates the fluorescent intensity $FCA_1$ for a case containing the elements $J_0$ to $J_M$, where the radiation is excited by the line $L_{II}$, and emitted as characteristic radiation of the element $J_{JA}$.
4.10 **SUBROUTINE CALI** (J0, JM, JJA, AIT, SWITCH, FQCF, FQCA)

Calculates the total emergent intensity, AIT, of the line of the element JJA, for a case containing the elements J0 to JM. CALI establishes the sequence of procedures involving the correction function (see Figure 1).

4.11 **FUNCTION EI(X)**

Calculates \( EI(x) = \int_{-\infty}^{x} \frac{e^t}{t} \, dt \), used for the integration of stopping power.

4.12 **SUBROUTINE AINP** (C, IJ, IIMAX, SD)

This subroutine is needed for the input of intensity data in any form except of k-values. If intensity data are on cards, this subroutine will be applicable as is. Other subroutines, such as PTLOAD subroutine which enters data from a magnetic tape into the UNIVAC 1108, can be used to prepare data for AINP. The subroutine PTLOAD is reproduced in the statements of the program, but not discussed elsewhere, since it is specifically designed for use with the UNIVAC 1108 computer.

Function DEADT, which performs the dead-time corrections for counts, is attached to subroutine AINP.

**Use of the Program**

In the present form, the program should be acceptable to all computers having a FORTRAN IV compiler. The executive command cards are, of course, specific for a system and must be adapted to it.
5. Statements of the Program
COR2

A CORRECTION PROGRAM FOR ELECTRON PROBE MICROANALYSIS
BY HENOC, HEINRICH, AND MYKLEBUST

MAIN PROGRAM

THIS SECTION HANDLES ALL INPUT AND OUTPUT. THE ANALYSIS METHOD IS DETERMINED HERE AND THE PROPER ORDER IS SET UP. THE ITERATION PROCEDURE IS ALSO HERE.

LOGICAL FIRST

INTEGER SWITCH

DIMENSION NCO(15),MF(15),A(100),WAV(12,100),CL(3,12,100),ZL(3,12,100),NZ(15),AK(15),LA(15),CSEC(15),C(15)
DIMENSION KM(100),LM(12,100),EXP0(15,15),CC(15,15),CI(100),ANK(100),R(12,100)
DIMENSION FCK12(100),FCK23(100),FCK13(100),OME(12,100),IMA(15),WAV
1E(120,15),EX(120,15),MESS(15,15)
DIMENSION KB(120,15),LR(120,15),WA(15),KA(15),JJJ(120,15),RRR(120,15),OEG(120,15)
DIMENSION FQF(15),FCF(15),FCASF(15),RF(15),NV(15),AI(15),AEIX(15)
1,CT(15),AIR(15),CD(100,15),SD(100,15),ELNA(100),LI(9,3),CON(15),FQ
2(15),FQCA(15)
13/EXP0,CC/B25/CI,ANK,ANKL,R/B126/FCK12,FCK23,FCK13,OME/B239/IMA,
2WAVE,RR,EX,MES/S/B129 KB,LR/BS/WA,KA,JJ,RRR,OMEG/B1C/ICF
COMMON /BINP/III,NTAPE/B1/TOUT,FQF,FCF,FCASF,RF
COMMON DATA (ELNA(KK),KK=3,92)/2HLI,2HBE,1HB,1HC,1HN,1HO,1HF,2HNE,2HNA,2H
1MG,2HAL,2HST,1HP,1HS,2HCL,1HA,1HX,2HCA,2HGC,1HTI,1HV,2HCR,2HMN,2HF
2E,2HC0,2HNI,2HCU,2HZN,2HCA,2HC0,2HAS,2HSE,2HBR,2HFR,2HRB,2HSR,1HY
32HZ0,2HNB,2HMO,2HTC,2HRU,2HRH,2HPD,2HAG,2HCD,2HIN,2HSN,2HNB,2HTE,1
4HS,2HXS,2HCS,2HBA,2HLA,2HCE,2HPR,2HND,2HMP,2HSM,2HEU,2HCD,2HTB,2HD
33,2HY0,2HER,2HTM,2HYB,2HLU,2HNF,2HTA,1HW,2HRE,2HOS,2HTR,2HPT,2HAU
42HY2,2HTL,2HFB,2HBI,2HP0,2HAT,2HRN,2HFR,2HRA,2HAC,2HTH,2HPA,1HU/
35/DATA LI(1,1)/3HKB1/LI(1,2)/3HKA/LI(1,3)/3HKA2/LI(2,1)/3HBL3/LI(2,12)/3HBL4/LI(3,1)/3HLG1/LI(3,2)/3HBL1/LI(4,1)/3HBL2/LI(4,2)/3HLA1/L
37/21(4,3)/3HLA2/LI(9,1)/3MLA1/LI(7,1)/3HMB1/

10 FORMAT (1I0.5,2HK,3H2,1H2H,=.F5.4)
20 FORMAT (1I0.5,19X,A2,1I1,11,5X,F6.4)
30 FORMAT (1I0.5,F3)
40 FORMAT (2I1,F6.3,3F6.4,F6.2,2F4.2)
50 FORMAT (F7.5,2F6.4,1I1)
60 FORMAT (2I1,2I1,3I1,68X,LI)
70 FORMAT (F7.5,6F6.4)
80 FORMAT (I2,10X,F7.3,2I1,F6.4,2I1,F6.4)
90 FORMAT (I2,F5.4)
100 FORMAT (15F5.4)
110 FORMAT (12,10X,1F5.4)
120 FORMAT (/THEELEMENT,12.4X,9HATOMIC NO,1I2,3/30X,9HABS COEFF,3/30X,5H(1K)=.F8.2,3X,5HK(1K)=.F8.2)
130 FORMAT (18H COMP STANDARD/5H JJA=12,4X,4H1NZA=12(4X,9H3NZ((1I2,12H)=12,4X,4H1NZ(3X,F5.3,3X,3HCC=.F8.2,3X,5HEXP0=.F4.2))
140 FORMAT (11X,4H1AIR(11,12H)=.F6.4)
150 FORMAT (/12X,3HAI(11,12H)=.E10.5)
160 FORMAT (/10H0,10H SAMPLE NO,1I3,5X,9HSTANDARDS)
170 FORMAT (/7X,8HPOINT NO,1I2)
180 FORMAT (/7X,13HITERATION NO,1I2)
READ DATA INTO THE ELEMENT TABLE

READ (5,30) NELM
DO 350 NEC=1,NELM
READ (5,40) J,KM(J),A(J),FCK12(J),FCK23(J),FCK13(J),CI(J),ANK(J),A
KJ=KM(J)
DO 350 K=1,KMJ
READ (5,50) WAV(K,J),R(K,J),OME(K,J),LM(K,J)
LMKJ=LM(K,J)
IF (LMKJ.EQ.0) GO TO 350
READ (5,70) (CL(L,K,J),ZL(L,K,J),L=1,LMKJ)
350 CONTINUE

READ IN INITIAL DATA FOR EACH SAMPLE

READ (5,30) NECM
DO 1010 NEC=1,NECM
NIT=0
KSTOP=1
360 READ (5,60) JJM, JJAM, ND, NPM, LOUT, ICOF, FIRST
NP1=NPM-1
IF (.NOT.FIRST) GO TO 360
READ (5,290)
SWITCH=0
WRITE (6,300)
WRITE (6,290)
WRITE (6,160) NEC
DO 430 JJA=1,JJAM
CON(JJA)=0.
370 CONTINUE

READ ELEMENT CARDS FOR EACH SAMPLE

READ (5,80) NZ(JJA),EO,KA(JJA),LA(JJA),COSEC(JJA),NV(JJA),NEST,CON
1(JJA)
NCO(JJA)=1
WA(JJA)=12.398/EO
C(JJA)=1.
CALCULATE FLUORESCENCE CONSTANTS FOR PURE ELEMENTS

CALL COCA (JJA, JJA, JJA)
IF (LOUT.EQ.0) GO TO 370
WRITE (6,120) JJA, NZ(JJA), CC(JJA, JJA), EXPO(JJA, JJA)
CONTINUE
IF (NCO(JJA).EQ.0) GO TO 1010
NZA=NZ(JJA)
KAA=KA(JJA)
LAA=LA(JJA)
IF (NZA.LT.10) LAA=2
IF (NZA.LT.40.AND.KAA.EQ.4) LAA=2
WRITE (6,280) ELNA(NZA), LI(KAA, LAA)

CALCULATION OF ABSORPTION, ATOMIC NUMBER, AND CONTINUUM

FLUORESCENCE CORRECTIONS FOR THE STANDARDS.

AI = THE TOTAL CORRECTION FACTOR

CALL CALI (JJA, JJA, JJA, AIT, SWITCH, FQC, FQCA)
IF (KSTOP.EQ.0) GO TO 1010
AI(JJA)=AIT
AIR(JJA)=1.
IF (LOUT.EQ.0) GO TO 380
WRITE (6,150) JJA, AI(JJA)

READ DATA INPUT FOR COMPOUND STANDARDS AND CALCULATE

FLUORESCENCE CONSTANTS FOR THE COMPOUND STANDARDS.

READ (5,100) C(JJA)
JST=JJA+NEST
JJAS=JJA+1
READ (5,90) (NZ(JJ), C(JJ), JJ=JJAS, JST)
CALL COCA (JJA, JST, JJA)
IF (LOUT.EQ.0) GO TO 390
WRITE (6,130) JJA, NZ(JJA), (JJ, NZ(JJ), C(JJ), CC(JJ, JJA), EXPO(JJ, JJA)
1,JJ=JJA, JST)
GO TO 400
WRITE (6,240) JJA
CONTINUE
IF (NCO(JJA).EQ.0) GO TO 1010

CALCULATE CORRECTIONS FOR COMPOUND STANDARDS.

AIR = TOTAL CORRECTION

CALL CALI (JJA, JST, JJA, AIT, SWITCH, FQC, FQCA)
IF (KSTOP.EQ.0) GO TO 1010
AIR(JJA)=AIT/AI(JJA)
IF (LOUT.EQ.0) GO TO 420
WRITE (6,140) JJA, AIR(JJA)
CONTINUE

SORTING ROUTINE FOR ANALYSIS METHOD - NSW DETERMINES METHOD

1 - ALL ELEMENTS ANALYZED
2 - ONE ELEMENT BY STOICHIOMETRY
3 - ONE ELEMENT BY DIFFERENCE
4 - TWO OR MORE ELEMENTS NOT ANALYZED
5 - CALCULATE K-VALUES FROM KNOWN CONCENTRATIONS
JJA1=JJAM+1
IF (JJM-JJA1) 480, 450, 440
NSW=4
READ (5,110) (NZ(JJ), NV(JJ), CD(1, JJ), JJ=JJA1, JJM)
IF (CD(1, JJA1).GT.1.E-7) GO TO 460
IF (NV(JJA1).EQ.0) GO TO 470
IF ((JJM-JJA1).NE.0) GO TO 490
NSW=2
GO TO 490
NSW=5
GO TO 490
NSW=3
GO TO 490
NSW=1
DO 500 JJA=1, JJAM
  CALCULATE FLUORESCENCE CONSTANTS FOR UNKNOWNS
  CALL COCA (1, JJM, JJA)
  IF (NCO(JJA).EQ.0) GO TO 1010
  CONTINUE
  SWITCH=1
  IF (ND.EQ.1) GO TO 530

  READ IN K-VALUES FROM CARDS
  DO 510 NP=1, NPM
  READ (5,100) (CD(NP, JJA), JJA=1, JJAM)
  IF (NSW.NE.5) GO TO 540
  IF (NPM.EQ.1) GO TO 540
  DO 520 NP=2, NPM
  READ (5,100) (CD(NP, JJ), JJ=JJA1, JJM)
  GO TO 540

  DATA ARE READ BY THE INPUT SUBROUTINE (AINP)
  CALL AINP (CD, NPM, JJAM, SD)
  NP1=NPM-1

  BEGIN CALCULATION OF CONCENTRATIONS FOR EACH UNKNOWN
  DO 1000 NP=1, NPM
  NIT=0
  SC=0.0
  DO 550 JJA=1, JJAM
  C(JJA)=CD(NP, JJA)*AIR(JJA)
  IF (CON(JJA).GT.1.0E-7) C(JJA)=CD(NP, JJA)
  AKEX(JJA)=C(JJA)
  SC=SC+C(JJA)
  CONTINUE
  IF (NSW.EQ.5) SC=SC+CD(1, JJA1)
  GO TO (630, 560, 590, 590, 610), NSW

  STOICHIOMETRY CALCULATION
  C(JJA1)=0.0
  NZ0=NZ(JJA1)
  DO 570 JJA=1, JJAM
  NZA=NZ(JJA)
  CO=C(JJA)/A(NZA)*A(NZ0)*NV(JJA)/NV(JJA1)
C(JJA1) = C(JJA1) + C0

CONTINUE

SC = SC + C(JJA1)
GO TO 630

CALCULATE ONE ELEMENT BY DIFFERENCE

C(JJA1) = 1. - SC
SC = 1.
GO TO 630

TWO OR MORE ELEMENTS NOT ANALYZED

C(JJM) = 0.0
NZO = NZ(JJM)
NZEX = NZ(JJA1)
DO 600 JJA = 1, JJAM
NZA = NZ(JJA)
CO = C(JJA) / A(NZA) * A(NZO) * NV(JJA) / NV(JJM)
C(JJM) = C(JJM) + CO
CONTINUE

SC = SC + C(JJM)

C(JJM) = (1. - SC) * A(NZEX) * NV(JJM) / (A(NZEX) * NV(JJM) + A(NZO) * NV(JJA1))
C(JJM) = C(JJM) + (1. - SC) * A(NZO) * NV(JJA1) / (A(NZEX) * NV(JJM) + A(NZO) * NV(JJA1))
SC = 1.
GO TO 630

CALCULATE K-VALUES FROM KNOWN CONCENTRATIONS

DO 620 JJ = JJA1, JJM
C(JJ) = CD(NP, JJ)
CONTINUE

WRITE (6, 170) NP
DO 640 JJ = 1, JJAM
WRITE (6, 10) JJ, C(JJ)
CONTINUE

DO 650 JJ = 1, JJM
C(JJ) = C(JJ) / SC
CONTINUE

NSW2 = 2

START OF ITERATION LOOP

GO TO (840, 670), NSW2

IF (NIT.GT.20) GO TO 840
IF (LOUT.EQ.0) GO TO 680
WRITE (6, 180) NIT
CONTINUE

IF (NSW.NE.5) SC = 0.0
DO 730 JJA = 1, JJAM
IF (CD(NP, JJA), LT 1.0E-7) GO TO 720
IF (LOUT.EQ.0) GO TO 700
IF (NIT.EQ.0) GO TO 690
GO TO 700
WRITE (6, 190) JJA, NZ(JJA), (JJ, NZ(JJ), C(JJ), CC(JJ, JJA), Expo(JJ, JJA), 1, JJ = 1, JJM)

CALL CALI (1, JJM, JJA, AIT, SWITCH, FQC, FQCA)
IF (KSTOP.EQ.0) GO TO 1010
CT(JJA)=AIT/AI(JJA)
IF (CON(JJA).GT.1.0E-7) CT(JJA)=CD(NP,JJA)
IF (LOUT.EQ.0) GO TO 710
IF (NIT.EQ.0) WRITE (6,200) JJA,CT(JJA)
CONTINUE
IF (NSW.EQ.5) GO TO 730
CT(JJA)=AKEX(JJA)*C(JJA)*(1.-CT(JJA))/AKEX(JJA)*C(JJA)-CT(JJA)+1
IF (CON(JJA).GT.1.0E-7) CT(JJA)=CD(NP,JJA)
SC=SC+CT(JJA)
GO TO 730
CT(JJA)=0.
CONTINUE
IF (NSW.EQ.5) GO TO 730
CT(JJA)=1.-SC
END OF ITERATION LOOP - IF CONVERGENT, BEGIN WRITING OUTPUT
GO TO 660
WRITE (6,330)
DO 830 JJA=1,JJAM
C
C HYPERBOLIC APPROXIMATION FOR CONCENTRATIONS
C
CT(JJA)=AKEX(JJA)*C(JJA)*(1.-CT(JJA))/(AKEX(JJA)*(C(JJA)-CT(JJA))+1
CT(JJA)*(1.-C(JJA))
SC=SC+CT(JJA)
GO TO 790,750,740,770,820), NSW
CT(JJA1)=1.-SC
SC=1.
GO TO 790
CT(JJM)=0.0
DO 780 JJA=1,JJAM
NZA=NZ(JJA)
CO=CT(JJA)/A(NZA)*A(NZA)*NV(JJA)/NV(JJA1)
CT(JJA1)=CT(JJA1)+CO
CONTINUE
SC=SC+CT(JJA1)
GO TO 790
CT(JJM)=0.0
DO 780 JJA=1,JJAM
NZA=NZ(JJA)
CO=CT(JJA)/A(NZA)*A(NZA)*NV(JJA)/NV(JJM)
CT(JJM)=CT(JJM)+CO
CONTINUE
SC=SC+CT(JJM)
CT(JJA1)=1.-SC)*A(NZX)*NV(JJM)/(A(NZX)*NV(JJM)+A(NZX)*NV(JJ1))
CT(JJM)=CT(JJM)+(1.-SC)*A(NZX)*NV(JJM)/(A(NZX)*NV(JJM)+A(NZX)*NV)
1(JJA1))
SC=1.
90 NSW2=1
IF (LOUT.EQ.0) GO TO 800
WRITE (6,210) (JJ,CT(JJ),JJ=1,JJM)
CONTINUE
DO 810 JJA=1,JJAM
CT(JJA)=CT(JJA)/SC
IF (CON(JJA).GT.1.0E-7) CT(JJA)=CD(NP,JJA)
IF (ABS(CT(JJA)-C(JJA)).GT.1.E-5) NSW2=2
C(JJA)=CT(JJA)
CONTINUE
C(JJA1)=CT(JJA1)/SC
JJA2=JJA1+1
C(JJA2)=CT(JJA2)/SC
NIT=NIT+1
END
C
C END OF ITERATION LOOP - IF CONVERGENT, BEGIN WRITING OUTPUT
GO TO 660
WRITE (6,330)
DO 830 JJA=1,JJAM
31
HYPERBOLIC APPROXIMATION FOR K-VALUES

\[ CT(JJA) = \frac{1}{(1 + (1/AKEX(JJA) - 1) \times (1/CT(JJA) - 1)/(1/C(JJA) - 1))} \]

830 CONTINUE
840 WRITE (6,250)
     SACO=0.
     DO 870 JJ=1,JJM
        IF (NSW.EQ.5) GO TO 860
        IF (CON(JJ).GT.1.0E-7) GO TO 860
        IF (JJ.EQ.JJM) GO TO 860
        CT(JJ)=CT(JJ)*SC
     CONTINUE
890 DO 970 JJ=1,JJM
     NZA=NZ(JJ)
     SACH=SACO+CT(JJ)/A(NZA)
     JJMX=JJM
     CONTINUE
910 IF (JJM=JJM) GO TO 940
920 IF (CT(JJ).GT.1.0E-7) GO TO 950
940 RPFX=0.
     FCFX=0.
     GO TO 970
950 RPFX=RPF(JJ)/(FQF(JJ)*CT(JJ))
     FCFX=FCF(JJ)/RPFX(JJ)
     IF (FCASF(JJ).GT.1.0E-12) GO TO 960
     WRITE (6,230) FQF(JJ),RPFX,FCFX,FQC(JJ)
     GO TO 970
960 FCASFX=FCASF(JJ)/RPFX(JJ)
     WRITE (6,270) FQF(JJ),RPFX,FCFX,FQC(JJ),FCASFX,FQCA(JJ)
970 CONTINUE
     WRITE (6,310) SC
     WRITE (6,260) NIT
     IF (NSW.NE.2) GO TO 1000
C
WRITE STOICHIOMETRY OUTPUT IF THIS OPTION WAS USED

WRITE (6,320)
     NZA1=NZ(JJM)
     DO 990 JJ=1,JJM
        NZA=NZ(JJ)
        STOIC=(A(NZA)*NV(JJM)+A(NZA1)*NV(JJ))/(A(NZA)*NV(JJM))*CT(JJ)
        NY=NV(JJM)
        NX=NV(JJ)
        IF (NX.LT.NY) GO TO 980
        IF (MOD(NX,NY).EQ.1) GO TO 980
        NX=NX/NY
        NY=1
C
WRITE (6,320)
Determine all the constants necessary for a calculation

- **SUBROUTINE COCA (JO, JM, JJA)**

- **FORMAT** (//34H NUMBER OF EDGES GE 12 ARGUMENTS, (I2, I1H, I2, I1H, I2, I1H)

- **FORMAT** (//34H EO GREATER THAN 30 KV, ARGUMENTS, (I2, I1H, I2, I1H, I2, I1H)

- **FORMAT** (3H R, (I2, I1H, I2, 28H) MISSING IN DATA, ARGUMENTS, (I2, I1H, I2, I1H, I2, 1H)

- **NCO(JJA)=1**

- **NSW3=1**

- **I=1**

- **I3=0**

- **NZA=NZ(JJA)**

- **WAA=W(A(JJA))**

- **KAA=KA(JJA)**

- **F12=FCK12(NZA)**

- **F23=FCK23(NZA)**

- **F13=FCK13(NZA)**

- **IF (WAA.GT.WAV(KAA,NZA)) WRITE (6,30) JO, JM, JJA**

- **DO 450 JJ=JO,JM**

- **I2=0**

- **MESS(JJ,JJA)=0**

- **J=NZ(JJ)**

- **KMJ=KM(J)**

- **IF (J.GT.50) GO TO 50**

**Initialization of factors for the calculation of mass absorption coefficients.**

- **EXP0(JJ,JJA)=ANK(J)**

- **GO TO 60**

- **EXP0(JJ,JJA)=ANKL(J)**

- **CC(JJ,JJA)=CI(J)**

- **DO 440 K=1,KMJ**

- **KR1=1+K/2+K/8-(K/3)*(K/5)+((K-8)*(K/8))2+K/10-(K/11)2**

- **KR2=1+K/2+K/5-(K/5)*(K/6)+K/9+(K/12)2**

- **K1=KRI-1-(K/10)4+(K/12)3**

- **IF (WAV(K,J).LE.1.E-6) GO TO 440**

- **IF (WAV(K,J).LE.WAA) GO TO 70**

- **IF (WAV(K,J).GT.WAV(KAA,NZA)) GO TO 450**

- **GO TO 140**
NNR=R(K,J)
IF (KRL.NE.7.AND.NNR.EQ.0) GO TO 560
GO TO (80,90,100,110,120,130,570), KRL
80 IF (J.GT.50) GO TO 440
CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)*WAV(K,J)**ANKL(J)/WAV(K,J)**ANK(J)
EXPO(JJ,JJA)=ANKL(J)
GO TO 440
90 CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)
GO TO 440
100 CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)*WAV(K,J)**EXPO(JJ,JJA)/WAV(K,J)**2.6
EXPO(JJ,JJA)=2.6
GO TO 440
110 CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)
MESS(JJ,JJA)=MESS(JJ,JJA)+1
GO TO 440
120 CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)*WAV(K,J)**2.6/WAV(K,J)**2.22
EXPO(JJ,JJA)=2.22
MESS(JJ,JJA)=0
GO TO 440
130 CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)
GO TO 440
C
DETERMINE JUMP RATIOS (R) AND EXPONENTS (N) NEEDED BY THE
CONTINUUM FLUORESCENCE CORRECTION
C
140 I2=I2+1
I=I+1
WAVE(I,JJA)=WAV(K,J)
JJJ(I,JJA)=JJ
RRR(I,JJA)=0.0
OME(I,JJA)=0.0
KB(I,JJA)=0
LB(I,JJA)=0
IF (I2.EQ.1) GO TO (190,200,210,220,230,240,250,570), KR2
GO TO (150,160,170,180,570), K1
150 RR(I,JJA)=R(K,J)
EX(I,JJA)=EX(I-1,JJA)
GO TO 260
160 RR(I,JJA)=R(K,J)*WAV(K,J)**2.6/WAV(K,J)**EX(I-1,JJA)
EX(I,JJA)=2.6
GO TO 260
170 RR(I,JJA)=R(K,J)
EX(I,JJA)=EX(I-1,JJA)
MESS(JJ,JJA)=MESS(JJ,JJA)+1
GO TO 260
180 RR(I,JJA)=R(K,J)*WAV(K,J)**2.22/WAV(K,J)**EX(I-1,JJA)
EX(I,JJA)=2.22
MESS(JJ,JJA)=0
GO TO 260
190 IF (J.GT.50) GO TO 600
RR(I,JJA)=R(K,J)*WAV(K,J)**ANKL(J)/WAV(K,J)**ANK(J)
EX(I,JJA)=ANKL(J)
GO TO 260
200 RR(I,JJA)=R(K,J)
EX(I,JJA)=EXPO(JJ,JJA)
GO TO 260
210 RR(I,JJA)=R(K,J)*WAV(K,J)**2.6/WAV(K,J)**EXPO(JJ,JJA)
EX(I,JJA)=2.6
GO TO 260
220 RR(I,JJA)=R(K,J)
EX(I,JJA)=2.6
GO TO 260
RR(I,JJA)=R(K,J)
EX(I,JJA)=2.6
MESS(JJ,JJA)=MESS(JJ,JJA)+1
GO TO 260
RR(I,JJA)=R(K,J)*WAV(K,J)**2.22/WAV(K,J)**2.6
EX(I,JJA)=2.22
MESS(JJ,JJA)=0
GO TO 260
RR(I,JJA)=R(K,J)
EX(I,JJA)=EXPO(JJ,JJA)
GO TO 260
IF (JJ.NE.JJA) GO TO 420
KAS=KAA-KAA/6-KAA/7-KAA/9
GO TO (270,280,290,300,580,380), KAS
C
EFFICIENCY RATIOS --
(R-1)/R FOR THE CONTINUUM FLUORESCENCE FOR K-LINES
C
270
RRR(1,JJA)=(R(K,J)-1.)/R(K,J)
OMEG(1,JJA)=OME(K,J)
GO TO 440
280
KK=K
GO TO (310,320,330,340,350,360,370), KK
290
KK=K+K/2
GO TO (310,320,330,340,350,360,370), KK
300
KK=(K+4)/6*3+K
GO TO (310,320,330,340,350,360,370), KK
310
WRITE (6,30) JO,JM,JJA
NSW3=2
RKR=1./R(K,J)
GO TO 440
C
(R-1)/R FACTORS FOR THE CONTINUUM FLUORESCENCE CORRECTION FOR
L- AND M-LINES
C
L1-EDGE
C
320
RRR(1,JJA)=(R(K,J)-1.)/R(K,J)
OMEG(1,JJA)=OME(K,J)
GO TO (440,410), NSW3
C
L2-EDGE
C
330
RRR(1,JJA)=(R(K+1,J)-1.)/R(K,J)/R(K+1,J)
OMEG(1,JJA)=OME(K+1,J)*((1.+F12*(R(K,J)-1.))*R(K+1,J)/(R(K+1,J)-1.))
GO TO (440,410), NSW3
340
RRR(I-1,JJA)=(R(K,J)-1.)/R(K,J)
OMEG(I-1,JJA)=OME(K,J)
GO TO 440
C
L3-EDGE
C
350
RRR(1,JJA)=(R(K+2,J)-1.)/R(K,J)/R(K+1,J)/R(K+2,J)
OMEG(1,JJA)=OME(K+2,J)*((1.+F12*F13*R(K+1,J)*R(K+2,J)*(R(K,J)-1.))/(R(K+1, J)-1.))+F23*F22*(R(K+2,J)*(R(K+1,J)-1.))/(R(K+2,J)-1.))+F12*R(K+1,J)*R(K+ 1,J)*R(K+1,J)-1.)/(R(K+2,J)-1.))+F23*(R(K+2,J)*(R(K+1,J)-1.))/(R(K+2,J)-1.))
GO TO (440,410), NSW3
360
RRR(I-1,JJA)=(R(K+1,J)-1.)/R(K,J)/R(K+1,J)
OMEG(I-1,JJA)=OME(K+1,J)*((1.+F23*(R(K,J)-1.))*R(K+1,J)/(R(K+1,J)-1.))
GO TO 440

35
370 GO TO 440
380 RRR(I-1,JJA)=R(K,J)-1./R(K,J)
OMEG(I-1,JJA)=OME(K,J)
GO TO 440

C
C M5 - M5 EDGES

C
380 IF (K.EQ.1) WRITE (6,30) J0,JM,JJA
RRR=R(KAA,J)-1.
DO 390 LLL=K,KAA
RRR=RRR/R(LLL,J)
390 CONTINUE
IF (I2.EQ.1) GO TO 400
RRR(I-1,JJA)=RRR
OMEG(I-1,JJA)=OMEG(1,JJA)
GO TO 440

400 OMEG(1,JJA)=OME(KAA,J)
RRR(1,JJA)=RRR
GO TO 440
410 RRR(I-1,JJA)=RRR(1,JJA)
OMEG(I-1,JJA)=OMEG(1,JJA)
RRR(1,JJA)=RRR(1,JJA)*RKR
NSW3=1
GO TO 440
420 LMKJ=LM(K,J)
IF (LMKJ.EQ.0) GO TO 440
DO 430 L=1,LMKJ

C
C TEST FOR ANY CHARACTERISTIC FLUORESCENCE
C
IF THERE IS A CHARACTERISTIC FLUORESCENCE CORRECTION, THEN
DETERMINE THE (R-1)/R, FLUORESCENT YIELD, LINE NUMBER, EDGE
NUMBER, ELEMENT NUMBER, AND WAVELENGTH FOR THE PARTICULAR
CORRECTION.

C
IF (CL(L,K,J).GT.WAV(KAA,NZA).OR.CL(L,K,J)/WAV(KAA,NZA).LT.0.5) GO
1 TO 430
I=I+1
I3=I3+1
RRR(I,JJA)=0.0
OMEG(I,JJA)=0.0
WAVE(I,JJA)=CL(L,K,J)
JJJ(I,JJA)=JJ
EX(I,JJA)=EX(I-1,JJA)
KB(I,JJA)=K
LB(I,JJA)=L
430 CONTINUE
440 CONTINUE
450 CONTINUE
WAVE(1,JJA)=WAA
JJJ(1,JJA)=0
RR(1,JJA)=0.
EX(1,JJA)=0.
LB(1,JJA)=0
KB(1,JJA)=0
IM=I
I3M=I3
IM1=IM-1
IF (IM1.LT.2) GO TO 550
DO 480 I=2,IM1
IL=IM-I+1
480 continue
DO 470 II=2, IM1
IF (WAVE(II,JJA).GT.WAVE(II+1,JJA)) GO TO 460
GO TO 470
T1=WAVE(II,JJA)
T2=RR(II,JJA)
T3=JJJ(II,JJA)
T4=RRR(II,JJA)
T5=OMEG(II,JJA)
T6=EX(II,JJA)
T7=KB(II,JJA)
T8=LB(II,JJA)
WAVE(II,JJA)=WAVE(II+1,JJA)
RR(II,JJA)=RR(II+1,JJA)
JJJ(II,JJA)=JJJ(II+1,JJA)
RRR(II,JJA)=RRR(II+1,JJA)
OMEG(II,JJA)=OMEG(II+1,JJA)
EX(II,JJA)=EX(II+1,JJA)
KB(II,JJA)=KB(II+1,JJA)
LB(II,JJA)=LB(II+1,JJA)
GO TO 470

DO 500 I=2, IM1
IF (RRR(I,JJA).LE.1.E-7) GO TO 490
GO TO 500
RRR(I,JJA)=RRR(I-1,JJA)
OMEG(I,JJA)=OMEG(I-1,JJA)
CONTINUE
M4=IM1
I=2

IF (LB(I,JJA).EQ.0) GO TO 530
T1=WAVE(I,JJA)
T2=JJJ(I,JJA)
T3=KB(I,JJA)
T4=LB(I,JJA)
T5=RRR(I,JJA)
T6=OMEG(I,JJA)
DO 520 II=I,M4
WAVE(II,JJA)=WAVE(II+1,JJA)
RR(II,JJA)=RR(II+1,JJA)
JJJ(II,JJA)=JJJ(II+1,JJA)
RRR(II,JJA)=RRR(II+1,JJA)
OMEG(II,JJA)=OMEG(II+1,JJA)
EX(II,JJA)=EX(II+1,JJA)
KB(II,JJA)=KB(II+1,JJA)
LB(II,JJA)=LB(II+1,JJA)
CONTINUE

WAVE(M4+1,JJA)=T1
JJJ(M4+1,JJA)=T2
KB(M4+1,JJA)=T3
LB(M4+1,JJA)=T4
RRR(M4+1,JJA)=T5
OMEG(M4+1,JJA)=T6
M4=M4-1
GO TO 540

I=I+1

540 IF (I.LE.M4) GO TO 510

IMA(JJA)=IM-I3M

C

SET THE SWITCH FOR THE CHARACTERISTIC FLUORESCENCE CORRECTION

C

MF(JJA)=I3M

GO TO 620

560 WRITE (6,40) K,J,JO,JM,JJA

GO TO 610

570 WRITE (6,10) JO,JM,JJA,J,K

GO TO 610

580 WRITE (6,590)

GO TO 620

WRITE (6,40)

K,J,JO,JM,JJA

GO TO 610

WRITE (6,10)

JO,JM,JJA,J,K

GO TO 610

WRITE (6,590)

1H,'NO PROVISION IS MADE FOR LINES ORIGINATING'/')

GO TO 560

WRITE (6,20)

JO,JM,JJA

NCO(JJA)=0

IMA(JJA)=I

MF(JJA)=0

RETURN

END

SUBROUTINE CO (JO,JM,JJA,FC,FQC)

C

CALCULATION OF CONTINUUM FLUORESCENCE CORRECTION

C

DIMENSION N2(15),N4(15),D5(100),D6(12,100),CL(3,12,10),ZL(3,12,10)

DIMENSION EXPO(15,15),CC(15,15)

DIMENSION IMA(15),WAVE(120,15),RR(120,15),EX(120,15),MESS(15,15)

DIMENSION WA(15),KAA(15),LAA(15)

WAVE(1,JO,JM,JJA)

ZMK=0.

ACS=0.

RRRI=RRR(1,JJA)

OMEGI=OMEG(1,JJA)

DO 10 J=JO,JM

EXO(J)=EXPO(J,JJA)

CCO(J)=CC(J,JJA)

I=NZ(J)

C

CALCULATE CONSTANTS FOR CONTINUUM FLUORESCENCE

C

ACS=ACS+C(J)*AC(CL(LAA,KAA,NZA),I)*COS(JJA)

ANZ=NZ(J)

AK(J)=3.0E-5

ZMK=ZMK+C(J)*ANZ*AK(J)

CONTINUE

DO 70 I=1,IM1

DO 40 J=JO,JM

IF (J.EQ.JJJ(I,JJA)) GO TO 20
C 39
GO TO 40
C 40
EXO(J)=EX(I,JJA)
C 41
CCO(J)=CCO(J)/RR(I,JJA)
C 42
IF (J.EQ.JJA) GO TO 30
C 43
GO TO 40
C 44
OMEGI=OMEG(I,JJA)
C 45
RRRI=RRR(I,JJA)
C 46
CONTINUE
C 47

SET UP INTERVALS FOR NUMERICAL INTEGRATION
C 48
NIN2=(WAVE(I+1,JJA)-WAVE(I,JJA))/0.02
C 49
NIN=2*NIN2
C 50
H=0.01
C 51
IF (NIN.GE.10) GO TO 50
C 52
H=(WAVE(I+1,JJA)-WAVE(I,JJA))/10.
C 53
NIN=10
C 54
ANIN=NIN
C 55
RL=(WAVE(I+1,JJA)-WAVE(I,JJA))-ANIN*H
C 56
BO=WAVE(I,JJA)+RL
C 57
BN=WAVE(I+1,JJA)
C 58
BN1=BN-H
C 59
LKM=NIN-3
C 60

NUMERICAL INTEGRATION BETWEEN ABSORPTION EDGES
TRAPEZOIDAL RULE
C 61
S=0.5*(F(WAVE(I,JJA))+F(BO,J0,JM,JJA))*RL
C 62
SO=0.5*(FT(WAVE(I,JJA))+FT(BO))*RL
C 63

SIMPSONS RULE
C 64
S=S+H*(F(BO,J0,JM,JJA)+F(BN,J0,JM,JJA)+4.*F(BN1,J0,JM,JJA))/3.
C 65
SO=SO+H*(FT(BO)+FT(BN)+4.*FT(BN1))/3.
C 66
DO 60 LK=1,LKM,2
C 67
ALK=LK
C 68
BK1=BO+ALK*H
C 69
BK2=BK1+H
C 70
S=S+2.*[(2.*F(BK1,J0,JM,JJA)+F(BK2,J0,JM,JJA))*H/3.
C 71
SO=SO+2.*[(2.*FT(BK1)+FT(BK2))*H/3.
C 72
CONTINUE
C 73
EABI=0.5*ZL(LAA,KAA,NZA)*ZMK*C(JJA)*OMEGI*RRRI
C 74
FI=EABI*S
C 75
FIO=EABI*SO
C 76

FINAL VALUES OF EMITTED AND GENERATED CONTINUUM FLUORESCENCE
C 77
FC=FC+FI
C 78
FCO=FCO+FIO
C 79
CONTINUE
C 80

F(X) OF THE CONTINUUM
C 81
FQC=FC/FCO
C 82
RETURN
C 83
END
C 84
FUNCTION F (X,J0,JM,JJA)
C 85

CALCULATION OF THE INTEGRAL OF THE CONTINUUM CORRECTION FOR
THE EMITTED X-RAYS
C 86


DIMENSION N2(15),N4(15),D5(100),D6(12,100),D7(3,12,100),D8(3,12,10),N9(15),D10(15),N11(15),D12(15),C(15)
DIMENSION EX0(15),CCO(15)
COMMON N1,N2,N3,N4,D5,D6,D7,D8,N9,D10,N11,D12,C/B34/EX0,CC0,WAA,AC
1S/B410/ACAX,ACX
ACAX=CCO(JJA)***EXO(JJA)
ACX=0.0
DO 10 J=J0,JM
ACX=ACX+C(J)*CCO(J)***EXO(J)
CONTINUE
F=ACAX/ACS*(X-WAA)/WAA/X/X*ALOG(1.+ACS/ACX)
RETURN
END
FUNCTION AC(CL,J)

CALCULATION OF THE MASS ABSORPTION COEFFICIENTS

DIMENSION N1(15),N3(15),D4(100),WAV(12,100),D5(3,12,100),D6(3,12,100),N7(15),D8(15),N9(15),D10(15),D11(15)
DIMENSION CI(IOO),ANK(100),ANKL(IOO),R(12,100)
COMMON KSTOP,N1,N2,N3,D4,WAV,D5,D6,N7,D8,N9,D10,D11/B125/CI,ANK,ANKL,R
FORMAT (/4H MU(,F7.5,,1H,,I2,42H) UNKNOWN .MORE THAN 12 EDGES ARE 1 CROSSED)
20 FORMAT (/4H MU(,F7.5,,1H,,I2,14H) UNDEFINED,R(,,I2,1H,,I2,17H) MISSING IN DATA)

K=1

CONSTANTS FROM OPERATING POTENTIAL TO K-EDGE

CC=CI(J)
AN=ANK(J)
IF (CL.LT.WAV(K,J)) GO TO 100

CONSTANTS FROM K-EDGE TO L1-EDGE FOR ELEMENTS ATOMIC NUMBER 50 AND BELOW

IF (J.LE.50) CC=CC/R(K,J)*WAV(K,J)**(ANK(J)-ANKL(J))
AN=ANKL(J)
K=K+1
IF (WAV(K,J),LE.1.E-7) GO TO 30
IF (CL.LT.WAV(K,J)) GO TO 100
L=1+K/4-(K/4)*((K-1)/4)+(K/9)*4-(K/10)*2+(K/12)*4
NNR=R(K,J)
IF (L.NE.3.AND.NNR.EQ.0) GO TO 80
GO TO (40,50,60,70), L

ALL CONSTANTS ABOVE L1-EDGE

CC=CC/R(K,J)
GO TO 30

ALL CONSTANTS ABOVE L3-EDGE

CC=CC/R(K,J)
CC=CC*WAV(K,J)**(ANKL(J)-2.6)
AN=2.6
GO TO 30

ALL CONSTANTS ABOVE M5-EDGE

40
CALCULATION OF PRIMARY INTENSITIES

DIMENSION N2(15), N4(15), A(100), WAV(12, 100), D5(3, 12, 10), N7(15), D8(15), C(15)
DIMENSION FCK12(100), FCK23(100), FCK13(100), OME(12, 100)
COMMON N1, N2, N3, N4, A, WAV, D5, N7, D8, C/B126/FCK12, FCK23, FCK13, OME

PRA = 0.0
UO = WAV(KX, JX) / WAA
EM = 12.398 / WAV(KX, JX)
AM = 0.0
AMLW = 0.0
DO 10 J = JO, JM
I = NZ(J)
IF (I.EQ.JX) CX = C(J)
RZ = NZ(J)
AM = AM + C(J) * RZ / A(I)
CONTINUE

CALCULATE MEAN IONIZATION POTENTIAL - J

ZJ = 9.76 * RZ + 58.5 * (RZ ** (-.19))
AMLW = AMLW + C(J) * RZ / A(I) * ALOG(1166 * EM / ZJ)
CONTINUE

ALW = LN(V)  AW = V  ALUOW = LN(UO) = LN(UO) + LN(V)
ALW = AMLW / AM
AW = EXP(ALW)
ALUOW = ALOG(UO) + ALW
T1 = (EI(ALUOW) - EI(ALW)) * ALW / AW

T2 = THE INTEGRATED VOLTAGE DEPENDENT TERM

T2 = (U0 - 1. - T1) * 0.76 * 0.5 / AM
IF (KX.GT.4) GO TO 90
GO TO (20, 30, 40, 60), KX

SELECT THE NUMBER OF ELECTRONS (ZNL) AND THE FLUORESCENT YIELD (OMED) FOR THE ABSORPTION EDGE PRODUCING THE MEASURED LINE

K-EDGE

ZNL = 2.
OMED = OME(KX, JX)
GO TO 130
L1-EDGE

30 ZNL=2.
OMED=OME(KX,JX)
GO TO 130

L2-EDGE

40 ZNL=2.
IF (WAV(KX-1,JX).GT.WAA) GO TO 50
OMED=OME(KX,JX)
GO TO 130
50 OMED=OME(KX,JX)*(1.+FCK12(JX))
GO TO 130

L3-EDGE

60 ZNL=4.
IF (WAV(KX-2,JX).GT.WAA) GO TO 80
IF (WAV(KX-1,JX).GT.WAA) GO TO 70
OMED=OME(KX,JX)
GO TO 130
70 OMED=OME(KX,JX)*(1.+0.5*FCK23(JX))
GO TO 130
80 OMED=OME(KX,JX)*(1.+0.5*FCK13(JX)+0.5*FCK23(JX)*(1.+FCK12(JX)))
GO TO 130

M-EDGES  NONE OF THE LISTED LINES ARE PRODUCED BY THE M1 AND M2-EDGES

90 KXX=1+(KX-4)/3+(KX-4)/5
OMED=OME(KX,JX)
GO TO (100,110,120), KXX

M3-EDGE

100 ZNL=2.
GO TO 130

M4-EDGE

110 ZNL=4.
GO TO 130

M5-EDGE

120 ZNL=6.
130 TO=OMED*ZL(LX,KX,JX)*CX*ZNL/A(JX)
PRA=TO*T2
RBA=0.0
DO 140 J=J0, JM
Z=NZ(J)
RBA=RBA+RB(UO,Z)*C(J)
CONTINUE

PRA = THE PRIMARY INTENSITY

PRA=PRA*RBA
RETURN
END

FUNCTION RB (UO,Z)
CALCULATION OF BACKSCATTER \(-R-\) FROM DUNCUMBS FIT

\[
\begin{align*}
W_1 &= \frac{1}{U_0} \\
W_2 &= W^2 \\
W_3 &= W^3 \\
W_4 &= W^4 \\
W_5 &= W^5 \\
Z_1 &= 1.0 \times 10^{-02} \times Z \\
Z_2 &= 1.0 \times 10^{-04} \times Z^2 \\
Z_3 &= 1.0 \times 10^{-06} \times Z^3 \\
Z_4 &= 1.0 \times 10^{-08} \times Z^4 \\
Z_5 &= 1.0 \times 10^{-10} \times Z^5 \\
R_1 &= -0.581 + 2.162 \times W - 5.137 \times W^2 + 9.213 \times W^3 - 8.619 \times W^4 + 2.962 \times W^5 \\
R_2 &= -1.589 - 8.108 \times W + 28.791 \times W^2 - 47.744 \times W^3 + 46.540 \times W^4 - 17.676 \times W^5 \\
R_3 &= 5.4 + 19.184 \times W - 75.733 \times W^2 + 120.05 \times W^3 - 110.70 \times W^4 + 41.792 \times W^5 \\
R_4 &= -5.712 - 21.645 \times W + 88.128 \times W^2 - 136.06 \times W^3 + 111.75 \times W^4 - 42.445 \times W^5 \\
R_5 &= 2.095 + 8.947 \times W - 36.51 \times W^2 + 55.694 \times W^3 - 46.079 \times W^4 + 15.851 \times W^5 \\
R_B &= 1 + R_1 \times Z_1 + R_2 \times Z_2 + R_3 \times Z_3 + R_4 \times Z_4 + R_5 \times Z_5 \\
\text{RETURN} \\
\text{END} \\
\end{align*}
\]

FUNCTION FQI (JO, JM, LX, KX, JX, WAA)

CALCULATION OF F(X)

\[
\begin{align*}
\text{DIMENSION N2}(15), N4(15), A(100), \text{WAV}(12,100), \text{CL}(3,12,10), D5(3,12,10), N7(15), D6(15), N7(15), \text{COSEC}(15), C(15) \\
H &= 0.0 \\
\text{ACS} &= 0.0 \\
\text{DO} 10 JJ=J0, JM \\
J &= \text{NZ}(JJ) \\
\text{IF} (J.EQ.JX) JJA=JJ \\
RZ &= \text{NZ}(JJ) \\
\text{CALCULATE THE H OF PHILIBERT AND THE VALUE OF CHI} \\
H &= H + 1.2 \times A(J) \times C(JJ) / RZ^2 \\
\text{ACS} &= ACS + C(JJ) \times A(C(LX,KX,JX), J) \times \text{COSEC}(JJA) \\
\text{CONTINUE} \\
\text{CALCULATE SIGMA AND FQI = F(X)} \\
\text{SIG} &= 4.5 \times 10^5 / (12.398 / \text{WAA})^1.65 - (12.398 / \text{WAV}(KX,JX))^1.65 \\
\text{FQI} &= (1 + H) / (1 + ACS / SIG) / (1 + H * (1 + ACS / SIG)) \\
\text{RETURN} \\
\text{END} \\
\end{align*}
\]

SUBROUTINE FCA (JO, JM, II, JJA, FCA1, FCA0)

CALCULATION OF CHARACTERISTIC FLUORESCENCE CORRECTION

\[
\begin{align*}
\text{DIMENSION N2}(15), N3(15), A(100), \text{WAV}(12,100), \text{CL}(3,12,10), \text{DZ}(3,12,10), N7(15), D6(15), N7(15), \text{COSEC}, C(15), \text{ZL}(3,12,10), \text{NZ}(15), D4(15), \text{LA}(15), \text{COSEC}(15), C(15), \text{CA}(2), \text{CB}(2) \\
\text{DIMENSION KB}(120,15), \text{LB}(120,15), \text{WA}(15), \text{KA}(15), JJJ(120,15), RRR(120,115), \text{OMEG}(120,15) \\
\text{DIMENSION FQF}(15), FCF(15), FCASF(15), RPF(15) \\
\text{COMMON N1,N2,N3, A, WAV, CL, ZL, NZ, D4, LA, COSEC, C/B5/P/WA, KA, JJJ, RRR, OMEG/B1289/KB, LB/LT/LOUT, FQF, FCF, FCASF, RPF} \\
\text{FORMAT (/13X,5HWA=,F7.5,4X,5HACBA=,F6.1,4X,4HACA=,F6.1,4X,4HACB=1,F6.1/(30X,4HCAI=,E10.5,14X,4HCBI=,E10.5))} \\
\text{NZA}=NZ(JJA) \\
\end{align*}
\]

43
KAA=KA(JJA)
LAA=LA(JJA)
JJB=JJJ(II,JJA)
NZB=NZ(JJB)
KBB=KB(II,JJA)
LBB=LB(II,JJA)

C ABSORPTION COEFFICIENT OF EXCITING RADIATION (B) IN THE
EXCITED ELEMENT (A)
ACBA=AC(CL(LBB,KBB,NZB),NZA)
H=0.0
ACA=0.0
ACB=0.0
DO 20 I=J0,JM
J=NZ(I)
RJ=J

C ABSORPTION COEFFICIENT OF RADIATION A IN THE SAMPLE X COSEC
THETA
ACA=ACA+AC(CL(LAA,KAA,NZA),J)*COSEC(JJA)*C(I)

C ABSORPTION COEFFICIENT OF RADIATION B IN THE SAMPLE
ACB=ACB+AC(CL(LBB,KBB,NZB),J)*C(I)
H=H+1.2*A(J)*C(I)/RJ**2
CONTINUE
SIG=4.5E05/((12.398/WA(JJA))**1.65-(12.398/WAV(KBB,NZB))**1.65)
FQIB=(1.+H)/(1.+ACA/SIG)/(1.+H*(1.+ACA/SIG))
CA(1)=(1.+H)*SIG
CA(2)=-CA(1)
CB(1)=SIG
CB(2)=SIG*(1.+1./H)

C CALCULATE CONSTANTS IN EQUATION AND THE PRIMARY INTENSITY
FCA1=OMEG(II,JJA)*RRR(II,JJA)*ZL(LAA,KAA,NZA)*ACBA*C(JJA)*0.5*PRA(1J0,JM,LBB,KBB,NZB,WA(JJA))
FCA0=FCA1/ACB

C S1 AND SO ARE THE INTEGRATIONS OF THE Emitted AND GENERATED
FACTORS RESPECTIVELY IN THE CRISS EQUATION
S2=FQIB*ALOG(1.+ACA/ACB)/ACA
IF (LOUT.EQ.O) GO TO 30
IF (NIT.EQ.O) WRITE (6,10) CL(LBB,KBB,NZB),ACBA,ACA,ACB,CA(1),CB(1)
30 CONTINUE
S1=0
SO=0
DO 40 I=1,2
S1=S1+CA(I)/(CB(I)+ACA)*ALOG(1.+CB(I)/ACB)/CB(I)
SO=SO+CA(I)/(CB(I)+ACA)*ALOG(1.+CB(I)/ACB)/CB(I)*ACB
40 CONTINUE

C FCA1 IS THE CHARACTERISTIC FLUORESCENCE FACTOR EMITTED
FCA1=FCA1*(S1+S2)
FCA0=FCA0*(SO+FQIB)
RETURN
END

SUBROUTINE CALI (JO, JM, JJA, AIT, SWITCH, FQCF, FQCA)  I  76-

DETERMINE SUBROUTINES TO BE CALLED TO CALCULATE THE TOTAL
EMITTED RADIATION FOR EITHER STANDARDS OR SAMPLES

INTEGER SWITCH

DIMENSION N2(15), MF(15), D3(100), D4(12, 100), D5(12, 10), J  
10, N2(15), D7(15), LA(15), D8(15), C(15), FQCF(15), FQCA(15)

DIMENSION KB(120, 15), LB(120, 15), WA(15), KA(15), JJJ(120, 15), RRR(120, 15)

DIMENSION IMA(15), WAVE(120, 15), RR(120, 15), EX(120, 15), MESS(15, 15)

DIMENSION FQF(15), FCF(15), FCFAF(15), RPF(15)

COMMON N1, N2, NIT, MF, D3, D4, D5, D6, NZ, D7, LA, D8, C/B1/23/IMA, WAVE, RR, EX

1, MESS/B5P/WA, KA, JJJ, RRR, OMEG/B1289/KB, LB/BLT/LOUT, FQF, FCF, FCFAF, RP
2F

COMMON /BICF/ IECOF

FORMAT (6X, 2HI=, I2, 3X, 5HWAVE=, F7.5, 3X, 3HRR=, F5.3, 3X, 4HJJA=, I2, 3X, 4  
1HRRR=, F5.3, 3X, 5HOME=, F5.3, 3X, 3HEX=, F5.3, 3X, 3HLB=, I1, 3X, 3K KB=, I1)  

FORMAT (/5H JJA=, I1, 8X, 3HRP=, E10.5, 3X, 3HFQ=, F6.4, 3X, 3HFC=, E10.5, 3X  
1, 4HFQC=, F6.4/)

FORMAT (71X, 5HFC=, E10.5, 2X, 6HFQCA=, F6.4)

FORMAT //6X, 5HMESS(, I2, 1H, , I2, 2H), =I2, 67H .M4 EDGE IS CROSSED, ABS

10RPTION COEFFICIENTS MAY NOT BE MEANINGFUL

FORMAT (1H+, 19X, 5HAT NO. I3, 4X, 5HF(X)=, F6.4, 4X, 14HI(P)/(F(X)*C)=, E1  
10.5, 4X, 10HI(C)/I(P)=, E10.5, 4X, 10HF(X), CONT=, F6.4)

IMAM=IMA(JJA)+MF(JJA)

IF (LOUT.EQ.0) GO TO 60

IF (NIT.EQ.0) WRITE (6, 10) (I, WAVE(I, JJA), RR(I, JJA), JJJ(I, JJA), RRR  
I(I, JJA), OMEG(I, JJA), EX(I, JJA), LB(I, JJA), KB(I, JJA), I=1, IMAM)

GO TO 60

CONTINUE

60

DO 70 JJ=JO, JM

IF (MESS(JJ, JJA).EQ.0) GO TO 70

WRITE (6, 40) JJ, JJA, MESS(JJ, JJA)

70

CONTINUE

70

IF (ICOF.EQ.1) GO TO 80

STOP

FC = EMITTED RADIATION DUE TO FLUORESCENCE BY THE CONTINUUM

CALL CO (JO, JM, JJA, FC, FQC)

GO TO 90

80

FC=0.

FQC=0.

90

RP=PR(A(JO, JM, LA(JJA), KA(JJA), NZ(JJA), WA(JJA))

FQ=FQI(JO, JM, LA(JJA), KA(JJA), NZ(JJA), WA(JJA))

RP = THE EMITTED PRIMARY INTENSITY

RP=RP*FQ

FCAS=0.0

FCF=0.0

IF (LOUT.EQ.0) GO TO 100

WRITE (6, 20) JJA, RP, FQ, FC, FQC

CONTINUE

FCFX=FC/RP

RPFX = THE NORMALIZED GENERATED PRIMARY INTENSITY

RPFX=RP/(FQ*FC(JJA))

45
WRITE DATA FOR STANDARDS
IF (SWITCH.EQ.0) WRITE (6,50) NZ(JJA),FQ,RPFX,FCFX,FQC
FQCF(JJA)=FQC
FQF(JJA)=FQ
FCF(JJA)=FC
RPF(JJA)=RP
IF (MF(JJA).EQ.0) GO TO 130

CHARACTERISTIC FLUORESCENCE CORRECTION - THE VALUE OF MF IS SET IN SUBROUTINE COCA

IO=IMA(JJA)+1
DO 120 I=IO,IMAM
CALL FCA(JO,JM,I,JJA,FCA1,FCA0)
IF (FCA0.LT.1.0E-12) GO TO 110
FCA1=FCA1/FCA0
IF (LOUT.EQ.0) GO TO 110
WRITE (6,30) FCA1,FQCA1
110 CONTINUE

FCAS = TOTAL EMITTED RADIATION DUE TO CHARACTERISTIC FLUORESCENCE
FCAS=FCAS+FCA1
FCAS0=FCAS0+FCA0
120 CONTINUE
IF (FCAS0.LT.1.0E-12) GO TO 130
FQCA(JJA)=FCAS/FCAS0

AIT = TOTAL EMITTED RADIATION

AIT=RP+FC+FCAS
FCASF(JJA)=FCAS
RETURN

FUNCTION EI (X)

EI=ALOG(X)+X
TN=X
N=1
AN=N
IF (AN.GT.2.*X.AND.TN.LT.1.E-06) GO TO 20
TN=TN*X*AN/(AN+1.)**2
EI=EI+TN
N=N+1
GO TO 10
20 RETURN
END

FUNCTION FT (X)

CALCULATION OF THE INTEGRAL OF THE CONTINUUM FLUORESCENCE CORRECTION FOR GENERATED X-RAYS

DIMENSION D1(15),D2(15)
COMMON /B34/ D1,D2,WAA,DACS/B410/ACAX,ACX
FT=ACAX/ACX*(X-WAA)/WAA/X/X
RETURN
END
SUBROUTINE AINP (C, IJ, IIMAX, SD)
DOUBLE PRECISION SUM, SSUM, SUNK, SFD
DIMENSION NUMBER (1000), NTABLE (100, 8), MCO (8), NCODE (100, 7), T (100), ICO
IN (7, 2), NSTD (12, 7, 2), SNSTD (7, 2), CST (7, 2), SPH (5, 7), SPHC (5, 7), PHC (5, 7)
C (100, 6), PEAK (7), KK (5), TIM (5), SD (100, 7), SUM (6, 7), SSUM (6, 7),
SDESC (6, 7), FSD (6, 7)
COMMON /BINPT/ III, NTAPE
FORMAT (12, I5, I2)
FORMAT (1018)
FORMAT (1H0, 8HELEMENT, 1.11H POINTS IS, F6.4)
FORMAT (1H0, 8HELEMENT, 10R, I2, 11H POINTS IS, F6.4)

READ DATA FROM MAG TAPE AND SET UP TABLE
READ (5, 10) NC, NM, NTC, NAV, ND, NTRA
NC1 = NC - 1
NS = 6
M = NC * ND
IF (NTC.EQ.1) GO TO 60
INDEX = 0
CALL PTLOAD (NUMBER, M, NS, NC)
DO 50 NROW = 1, ND
DO 50 NCOL = 1, NC
INDEX = INDEX + 1
NTABL (NROW, NCOL) = NUMBER (INDEX)
CONTINUE
GO TO 80

READ DATA FROM CARDS AND SET UP TABLE
DO 70 NROW = 1, ND
READ (5, 20) (NTABL (NROW, NCOL), NCOL = 1, NC)
CONTINUE
80 CONTINUE

SEPARATE MANUAL DATA ENTRY INTO 6 VARIABLES
DO 110 NROW = 1, ND
MCO (1) = NTABL (NROW, NM)
DO 100 I = 1, 6
IK = 6 - I
IF (MCO (I).EQ.0) GO TO 90
ITEN = 10 ** IK
IF (MCO (I).LT.ITEN) GO TO 90
NCODE (NROW, I) = MCO (I) / ITEN
IF (IK.EQ.0) GO TO 100
MCO (I+1) = MCO (I) - NCODE (NROW, I) * ITEN
GO TO 100
90 NCODE (NROW, I) = 0
MCO (I+1) = MCO (I)
CONTINUE
110 CONTINUE

SET UP TABLES OF STANDARDS AND BACKGROUNDS FOR ALL ELEMENTS
DO 130 I = 1, NC1
DO 120 J = 1, 2

47
SUM(I,J)=0
SSUM(I,J)=0
ICON(I,J)=0
SNSTD(I,J)=0
CONTINUE

DO 160 NROW=1,ND
   CONTINUE
   DO 150 I=1,NC1
      PHC(NROW,I)=0
      IF (NCODE(NROW,I).EQ.0) GO TO 150
      T(NROW)=1000
   CONTINUE
   CONTINUE
   DO 140 I=1,NC1
      IF (NCODE(NROW,I).NE.6) GO TO 150
      IC0N(I,1)=IC0N(I,1)+1
      IIC=IC0N(I,1)
      NSTD(IIC,1,I,1)=NROW
      GO TO 150
   CONTINUE
   IF (NCODE(NROW,I).NE.7) GO TO 150
   IC0N(I,2)=IC0N(I,2)+1
   IIC=IC0N(I,2)
   NSTD(IIC,1,I,2)=NROW
   GO TO 150
   CONTINUE
   CONTINUE
   CONTINUE
   CONTINUE
   CONTINUE
   CONTINUE

C AVERAGE STANDARDS AND BACKGROUNDS AND CORRECT FOR DEAD TIME

DO 200 I=1,NC1
   IF (ICON(I,J).EQ.0) GO TO 200
   IC=ICON(I,J)
   DO 170 IIC=1,IC
      NR=NSTD(IIC,1,I,J)
      SNSTD(I,J)=SNSTD(I,J)+NSTD(IIC,2,I,J)/(ICON(I,J)*T(NR))
   CONTINUE
   SUMS(I,J)=SUM(I,J)**2/ICON(I,J)
   ASUM=SUM(I,J)/ICON(I,J)
   SSTD=DSQRT((SUM(I,J)-SUMS(I,J))/(ICON(I,J)-1))/ASUM
   SSTSD=SNGL(SSTD)
   WRITE (6,30) I,ICON(I,J),SSTSD
   GO TO 180
   WRITE (6,40) I,ICON(I,J),SSTSD
C AVERAGE DATA ON INDIVIDUAL PHASES AND CORRECT FOR DEAD TIME

DO 250 I=1,NC1
   DO 210 J=1,5
      KK(J)=0
   CONTINUE
   SUM(J,I)=0
   SSUM(J,I)=0
   TIM(J)=0
   CONTINUE
SPH(J,I)=0
CONTINUE
DO 220 NROW=1,ND
IF (NCODE(NROW,I).EQ.0.OR.NCODE(NROW,I).GE.6) GO TO 220
J=NCODE(NROW,I)
KK(J)=KK(J)+1
SPH(J,I)=SPH(J,I)+NTABL(NROW,I)/T(NROW)
TIM(J)=TIM(J)+T(NROW)
SUM(J,I)=SUM(J,I)+NTABL(NROW,I)
SSUM(J,I)=SSUM(J,I)+NTABL(NROW,I)**2
CONTINUE
DO 220 J=1,5
SPHC(J,I)=DEADT(SPH(J,I)/KK(J),I,NIND)
IF (NTRA.EQ.1) GO TO 230
SPHC(J,I)=SPHC(J,I)*TIM(J)/KK(J)
CONTINUE
SUM(J,I)=SUM(J,I)**2/KK(J)
ASUM=SUM(J,I)/KK(J)
FSD(J,I)=DSQRT((SSUM(J,I)-SUMS(J,I))/(KK(J)-1))/ASUM
CONTINUE
CONTINUE
GO TO 290
C
C CORRECT FOR DEAD TIME ON INDIVIDUAL DETERMINATIONS
C
260 DO 280 NROW=1,ND
DO 270 I=1,NCI
IF (NCODE(NROW,I).EQ.0.OR.NCODE(NROW,I).GE.6) GO TO 270
PHC(NROW,I)=DEADT(NTABL(NROW,I)/T(NROW),I,NIND)
IF (NTRA.EQ.1) GO TO 270
PHC(NROW,I)=PHC(NROW,I)*T(NROW)
CONTINUE
280 CONTINUE
290 CONTINUE
GO TO 290
C
PEAK MINUS BACKGROUND ON STANDARDS
C
300 DO 300 I=1,NCI
IF (ICON(I,1).EQ.0) GO TO 300
PEAK(I)=CSTD(I,1)-CSTD(I,2)
CONTINUE
IF (NAV.EQ.1) GO TO 340
C
C DETERMINE K-VALUES ON AVERAGED PHASES
C
IJ=0
DO 330 J=1,5
II=0
DO 320 I=1,NCI
IF (SPHC(J,I)) 320,320,310
310 II=II+1
IF (II.EQ.1) IJ=IJ+1
C(IJ,II)=(SPHC(J,I)-CSTD(I,2))/PEAK(I)
SD(IJ,II)=SNGL(FSD(J,I))
IIMAX=II
320 CONTINUE
330 CONTINUE
RETURN
C
C DETERMINE K-VALUES ON INDIVIDUAL POINTS
C
CORRECTION OF RAW INTENSITIES FOR DEAD TIME

THIS MAY BE EXPANDED TO INCLUDE MORE THAN THE TWO DETECTORS
USED HERE

IF (NIND.EQ.0) GO TO 10
IF (IND.GT.NIND) GO TO 20

DEAD TIME OF FIRST DETECTOR

DEADT=COUNT/(1-COUNT*3.2E-6)
NIND=IND
GO TO 30

DEAD TIME OF SECOND DETECTOR

DEADT=COUNT/(1-COUNT*2.8E-6)
CONTINUE
RETURN

SUBROUTINE PTLOAD (NUMBER, M, NS, NC)

READ DATA FROM MAGNETIC TAPE - USE ONLY ON UNIVAC 1108 FORTRAN 5

COMMON /BINPT/, III, NTAPE
DIMENSION NUMBER(M), NEOF(1)/056/, ICHK(2)/040, 015/, IOR(10)/060, 061
1,062, 063, 064, 065, 066, 067, 070, 071/
DIMENSION FMT(2)
DATA (FMT(I).I=1,2)'/(1H , ', '9I10)'/
FORMAT (1H1)
20 FORMAT (1HO)
30 FORMAT (1HO,20X,'DIRECT LISTING OF DATA INPUT VIA PTLOAD')
IF (NC.GT.5) GO TO 40
FLD(0, 6, FMT(2))=FLD(6*NC, 6, '012345')
GO TO 50
40 FLD(0,6,FMT(2))=FLD(6*(NC-6),6,'678900')
CONTINUE
DO 60 I=1,M
60 NUMBER(I)=0
NTAPE=7
WRITE (6,10)
DO 130 I=1,M
130 ICOUNT=I
DO 120 J=1,NS
120 WRITE (6,10)
10 FORMAT (I10)
20 FORMAT (I10)
30 FORMAT (A1,20X,'DIRECT LISTING OF DATA INPUT VIA PTLOAD')
40 FORMAT (A80)
50 FORMAT (A80)
60 FORMAT (A80)
70 FORMAT (A80)
CALL CHAR (N)
IF (N.EQ.NEOF(1)) GO TO 140
IF (.NOT.(N.EQ.ICHK(1).OR.N.EQ.ICHK(2))) GO TO 90
IF (ICOUNT.EQ.1) GO TO 80
IF (ICOUNT.EQ.2) GO TO 70
NUMBER(I)=0
GO TO 130

DO 100 K=1,11
IF (K.EQ.11) NCHK=NCHK+1
IF (NCHK.EQ.5000) GO TO 160
IF (K.EQ.11) GO TO 80

IF (N.EQ.IOCT(K)) GO TO 110
CONTINUE
NUMBER(I)=NUMBER(I)*10+IABS(K-1)
ICOUNT=ICOUNT+1
CONTINUE
WRITE (6,30)
WRITE (6,20)
WRITE (6,FMT) (NUMBER(I),I=1,M)
GO TO 170

FORMAT (1H 'INPUT ERROR TERMINATION')
WRITE (6,150)
STOP
RETURN

SUBROUTINE CHAR (N)
COMMON /BINPT/ III,NTAPE
DIMENSION INCOME(510),INPUT(170)
IF (III.NE.510) GO TO 200
CALL NTRAN (NTAPE,2,170,INPUT,L)
IF (L+1),180
IF (L) 210
I=1
DO 190 J=1,510,3
INCOME(J)=(AND(FLD(6,6,INPUT(I)),7)*16)+(AND(FLD(0,6,INPUT(I)),15)
1)
INCOME(J+1)=(AND(FLD(18,6,INPUT(I)),7)*16)+(AND(FLD(12,6,INPUT(I))
1,15))
INCOME(J+2)=(AND(FLD(30,6,INPUT(I)),7)*16)+(AND(FLD(24,6,INPUT(I))
1,15))
I=I+1
III=0
200 III=III+1
N=INCOME(III)
RETURN
210 N=-1
RETURN
END

SUBROUTINE DEFTAB
FORMAT (1H1,9X,'DEFINITIONS OF HEADINGS USED IN OUTPUT')
FORMAT (1H,'F(X)',16X,'ABSORPTION CORRECTION FACTORS FOR EITHE
1R STANDARDS OR SAMPLES. ')
FORMAT (1H ,4X,'IF(P)/(F(X)*C)',7X,'PRIMARY X-RAY GENERATION FROM E
1THER STANDARD OR SAMPLE IN PHOTONS PER ELECTRON. ')
FORMAT (1H ,4X,'I(C)/I(P)',11X,'RATIO OF EMITTED X-RAYS EXCITED BY
1 THE CONTINUUM TO THE EMITTED PRIMARY X-RAYS. ')
FORMAT (1H ,4X,'F(X),CONT',11X,'ABSORPTION CORRECTION FACTOR FOR T
1HE CONTINUUM IN THE STANDARD. ')
FORMAT (1H ,4X,'F(X),CON',13X,'SAME AS F(X),CONT BUT FOR THE SAMPLE
'CHARACTERISTIC FLUORESCENCE CORRECTION FACTOR."

80 FORMAT (1H, 4X, 'F(X)CHA', 13X, 'ABSORPTION CORRECTION FACTOR FOR THE 1 CHARACTERISTIC FLUORESCENCE CORRECTION.')

90 FORMAT (1H, 4X, 'AT CONC', 13X, 'ATOM FRACTION. '/5X, 'WT CONC', 13X, 'MAS 1S FRACTION."

100 FORMAT (1H, 4X, 'STD DEV', 13X, 'STANDARD DEVIATION OF THE DATA - NOT 1 USED WHEN INPUT IS INTENSITY RATIOS."

110 FORMAT (1H, 4X, 'K(1)...K(N)', 9X, 'INTENSITY RATIOS."

120 FORMAT (1H, 4X, 'TOTAL', 15X, 'TOTAL OF MASS FRACTIONS OBTAINED."

130 FORMAT (1H, 4X, 'ITERATION NO', 8X, 'THE NUMBER OF ITERATIONS REQUIRE 1D FOR CONVERGENCE."

140 FORMAT (1H0, 9X, 'WHEN THE STOICHIOMETRY OPTION IS USED, '/9X, 'A TABL 1EOF THE FORMULAS OF THE POSTULATED '/9X, 'COMPounds, AND THEIR MASS 2FRACTIONS AS'/9X, 'FOUNd IN THE ANALYSIS IS PRINTED OUT.\\\\\\ 3)

WRITE (6, 10)
WRITE (6, 20)
WRITE (6, 30)
WRITE (6, 40)
WRITE (6, 50)
WRITE (6, 60)
WRITE (6, 70)
WRITE (6, 80)
WRITE (6, 90)
WRITE (6, 100)
WRITE (6, 110)
WRITE (6, 120)
WRITE (6, 130)
WRITE (6, 140)
RETURN
END
### Table of Formats for the Data Input Cards

<table>
<thead>
<tr>
<th>Card no.</th>
<th>When used</th>
<th>Cols.</th>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>always</td>
<td>1-3*</td>
<td>(I3)</td>
<td>Number of sets of data</td>
</tr>
<tr>
<td>2</td>
<td>always</td>
<td>1-2*</td>
<td>(I2)</td>
<td>Number of elements in case</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3-4*</td>
<td>(I2)</td>
<td>Number of elements analyzed</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5</td>
<td>(I1)</td>
<td>Blank-input is either k-values or known concentrations.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6-7*</td>
<td>(I2)</td>
<td>1 - input is raw data via subroutine AINP.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>9</td>
<td>(I1)</td>
<td>Number of data points</td>
</tr>
<tr>
<td></td>
<td></td>
<td>11</td>
<td>(I1)</td>
<td>Blank-normal output. 1 - extended output.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80</td>
<td>(A1)</td>
<td>Blank-normal calculation 1 - omits continuum correction Must contain a &quot;T&quot;</td>
</tr>
<tr>
<td>3</td>
<td>always</td>
<td>1-80</td>
<td>(80H)</td>
<td>Title - anything may be input</td>
</tr>
<tr>
<td>4</td>
<td>always</td>
<td>1-2*</td>
<td>(I2)</td>
<td>Atomic number of first element</td>
</tr>
<tr>
<td></td>
<td></td>
<td>13-19</td>
<td>(F7.3)</td>
<td>Operating kilovoltage</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>(I1)</td>
<td>Edge no. of measured line 1 - K-edge 2 - L- edge 3 - LII-edge 4 - LIII-edge 5 - M- edge</td>
</tr>
<tr>
<td></td>
<td></td>
<td>21</td>
<td>(I1)</td>
<td>Line no. associated with the edge. (Depends on element table)</td>
</tr>
</tbody>
</table>

* - Right justified in field
<table>
<thead>
<tr>
<th>Card no.</th>
<th>When used</th>
<th>Cols.</th>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>If K-edge:</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1 - $K_{\beta_1,3}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2 - $K_{\alpha_1}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>If $L_{III}$-edge:</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1 - $L_{\beta_2}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2 - $L_{\alpha_1}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>etc.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22-27</td>
<td>(F6.4)</td>
<td>Cosecant of the x-ray emergence angle.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>28</td>
<td>(I1)</td>
<td>Valence of element if one element is calculated by stoichiometry.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>29</td>
<td>(I1)</td>
<td>If a compound standard was used, enter the number of additional elements in the standard.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>30-35</td>
<td>(F6.4)</td>
<td>Any number greater than 0 will fix the concentration of this element at whatever value is entered on cards 6a.</td>
</tr>
<tr>
<td>5a(1)</td>
<td>Element was from a compound standard</td>
<td></td>
<td>(F5.4)</td>
<td>If present, must follow card 4. Weight fraction of analyzed element in compound standard.</td>
</tr>
<tr>
<td>Card no.</td>
<td>When used</td>
<td>Cols.</td>
<td>Format</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>-----------------------------------</td>
<td>-------</td>
<td>--------</td>
<td>---------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>5a(2)</td>
<td>Element was from a compound standard</td>
<td>1-2*</td>
<td>(I2)</td>
<td>If present, must follow card 5a(1). Atomic number of the other element in compound standard. Weight fraction of this element in compound standard. If more than one other element is present, this card is repeated for each.</td>
</tr>
<tr>
<td>5b</td>
<td>Element not analyzed</td>
<td>1-2*</td>
<td>(I2)</td>
<td>Atomic number of element.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>13</td>
<td>(I1)</td>
<td>Valence if calculation by stoichiometry. Blank - calculate by difference or stoichiometry. If the weight fraction of the element is input here, the program will calculate the k-value of all other elements.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>14-18</td>
<td>(F5.4)</td>
<td></td>
</tr>
<tr>
<td>6a</td>
<td>Input is either k-values or weight fractions</td>
<td>Fields of 5 (15F5.4)</td>
<td></td>
<td>The k-values or weight fractions for each element (element 1 is first, etc.) measured are on one card for each point.</td>
</tr>
<tr>
<td>6b(1)</td>
<td>Input is raw data through subroutine AINP</td>
<td>1-2*</td>
<td>(I2)</td>
<td>Total number of 6-digit numbers read per data point. (Max. of 6 plus code)</td>
</tr>
<tr>
<td>Card no.</td>
<td>When used</td>
<td>Cols.</td>
<td>Format</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>--------------------</td>
<td>-------</td>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3-4*</td>
<td>(12)</td>
<td>Position of manual data entry for coding the line. (Must be in the last position.)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5-6*</td>
<td>(12)</td>
<td>Blank - read data from magnetic tape via PTLOAD (or tape reading routine supplied by user). 1 - read data from cards.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7-8*</td>
<td>(12)</td>
<td>Blank - average data on each phase for each element. 1 - do each point individually.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>9-13*</td>
<td>(12)</td>
<td>Total number of lines of input including all samples and standards.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>14-15*</td>
<td>(12)</td>
<td>Blank - calculate k-values from total counts. 1 - calculate k-values from counts/sec.</td>
</tr>
</tbody>
</table>

If the data are read from magnetic tape, no further cards are required.

6b(2) Raw data read from cards. One card per line. 10 fields of 8* Raw data for each element, time in seconds, and the data code. (Data code must be in last column used.)
Example of the order of the data input cards.
The program is set up to handle six entries besides the data code. The data code is a 6-digit number and must be the last entry on any line. Each digit in the code identifies the contents of its respective field. (If the data code is in the seventh field, the first digit refers to the first field, the second to the second field, etc.) The codes have the following meanings:

<table>
<thead>
<tr>
<th>Code</th>
<th>Contents of field contains:</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Field empty or deleted in this calculation.</td>
</tr>
<tr>
<td>1-5</td>
<td>Data from specimen. (May code up to 5 separate points. See below.)</td>
</tr>
<tr>
<td>6</td>
<td>Standard for an element.</td>
</tr>
<tr>
<td>7</td>
<td>Background for an element.</td>
</tr>
<tr>
<td>8</td>
<td>Not used at present.</td>
</tr>
<tr>
<td>9</td>
<td>Time in tenths of seconds.</td>
</tr>
</tbody>
</table>

Data may be sent from AINP to the main program in two different ways. First, it may send k-values for each element at each data point in the usual manner. Or, if each phase analyzed was coded with a different number (phases 1-5 above), the program will calculate an average k-value for each element in each point and send only these values to the main program.

The data need not be in any specific order. All measurements on any particular standard will be averaged (peak value or background). Specimens and standards may be mixed in any way provided the data code is correct.
number of cases

Case 1.

number of elements in specimen
number of elements analyzed
number of data points

first card of a case T

Example of a typical analysis.
Case 2.

number of elements in specimen
number of elements analyzed
number of data points
mass fraction of element in compound standard

atomic number of other element in standard

mass fraction of this element in standard

same as previous three cards, but for second element
pure element standard for third element

fourth element calculated by stoichiometry

atomic number

valence

intensity ratios for elements 1, 2 & 3
7. Outputs

The output originally developed, now called output 2, or extended output, contains many intermediate results and parameters that are very useful for troubleshooting. For routine analysis, a more compact output called output 1 was developed. This output is also printed when output 2 is requested.

Notes on output 1:

1. It is preceded by a title, which can contain whatever identification is desired.

2. "Sample No" X gives the number of the "case".

3. Then follows information on the standards:

F(X) is the attenuation factor for primary emission. 
I(P)/(FX(X)*C) gives the emitted primary intensity (photons/electron) divided by the mass fraction of the emitting element. The ratio of this term for the standard over the term for the specimen gives the "atomic number correction factor". 
I(C)/I(P) gives the ratio of the emitted fluorescence excited by the continuum, over the emitted primary intensity.
F(X), CONT is the absorption correction factor for fluorescence by the continuum (f_c).

After indicating the number of the point, the program prints the k-values for the elements measured. Nothing is printed here for elements determined by difference or stoichiometry.

4. Next, the results are printed, one line per element. The headings have the same meaning as for the standards with the following additions:

   AT CONC: Atomic fraction of element in the specimen
   WT CONC: Weight fraction
   STD DEV: If there are several measurements made per point, the true calculated standard deviation is given. If the number of counts for a single measurement is input, the standard deviation is estimated, assuming a Poissonian distribution. If k-values are input, the program prints .0000.
CHAR FLUOR:  Emitted fluorescent intensity due to characteristic excitation, divided by emitted primary intensity.

F(X) CHA:  Absorption correction factor for fluorescence due to characteristic lines.

If there is no characteristic fluorescence of an element, nothing is printed under CHAR FLUOR or F(X) CHA.

5. After the list by elements, the total of calculated mass fractions is printed, as well as the number of iterations. In the case of stoichiometry, a table of mass fractions of oxides is appended.

Notes on output 2:

1. Output 2 is requested by punching 1 in column 9 of card 2 as described under Table of Options for Sample Input.

2. The variable names printed out by output 2 are the same as those in the Index of Terms and Symbols.
OUTPUT 1

The regular output is preceded, at the beginning of each run, by the following table, which is produced through subroutine DEFTAB.

<table>
<thead>
<tr>
<th>Definition</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>F(X)</td>
<td>Absorption correction factors for either standards or samples.</td>
</tr>
<tr>
<td>I(P)/(F(X)*C)</td>
<td>Primary X-ray generation from either standard or sample in photons per electron.</td>
</tr>
<tr>
<td>I(C)/I(P)</td>
<td>Ratio of emitted X-rays excited by the continuum to the emitted primary X-rays.</td>
</tr>
<tr>
<td>F(X)*CONT</td>
<td>Absorption correction factor for the continuum in the standard.</td>
</tr>
<tr>
<td>F(X)CON</td>
<td>Same as F(X)*CONT but for the sample.</td>
</tr>
<tr>
<td>CHAR FLUOR</td>
<td>Characteristic fluorescence correction factor.</td>
</tr>
<tr>
<td>F(X)CHA</td>
<td>Absorption correction factor for the characteristic fluorescence correction.</td>
</tr>
<tr>
<td>AT CONC</td>
<td>Atom fraction.</td>
</tr>
<tr>
<td>WT CONC</td>
<td>Mass fraction.</td>
</tr>
<tr>
<td>STD DEV</td>
<td>Standard deviation of the data - not used when input is intensity ratios.</td>
</tr>
<tr>
<td>K(1),..,K(N)</td>
<td>Intensity ratios.</td>
</tr>
<tr>
<td>TOTAL</td>
<td>Total of mass fractions obtained.</td>
</tr>
<tr>
<td>ITERATION NO</td>
<td>The number of iterations required for convergence.</td>
</tr>
</tbody>
</table>

When the stoichiometry option is used, a table of the formulas of the postulated compounds, and their mass fractions as found in the analysis is printed out.
CU K-ALPHA - AU L-ALPHA  20KV

SAMPLE NO 1

<table>
<thead>
<tr>
<th>ELEMENT</th>
<th>AT NO</th>
<th>WT CONC</th>
<th>STD DEV</th>
<th>F(X)</th>
<th>I(P)/(F(X)*C)</th>
<th>I(C)/I(P)</th>
<th>F(X)CON</th>
<th>CHAR FLOUR</th>
<th>F(X)CHA</th>
</tr>
</thead>
<tbody>
<tr>
<td>CUKA1</td>
<td>29</td>
<td>0.9710</td>
<td>0.0000</td>
<td>0.9710</td>
<td>1.1546-02</td>
<td>3.953-01</td>
<td>8969</td>
<td>6783</td>
<td></td>
</tr>
<tr>
<td>AI1A1</td>
<td>79</td>
<td>0.741</td>
<td>0.0000</td>
<td>0.741</td>
<td>0.3175-03</td>
<td>3.6730-01</td>
<td>9069</td>
<td></td>
<td>1115</td>
</tr>
</tbody>
</table>

POINT NO 1
K(1) = 0.8401
K(2) = 1.1570

TOTAL = 1.0063

ITERATION NO 3

POINT NO 2
K(1) = 0.3622
K(2) = 0.332

TOTAL = 1.0080

ITERATION NO 3

POINT NO 3
K(1) = 0.4634
K(2) = 0.5286

TOTAL = 1.0052

ITERATION NO 3

POINT NO 4
K(1) = 0.2464
K(2) = 0.7525

TOTAL = 1.0068

ITERATION NO 3
SPRINGWATER OLIVEF 20KV

SAMPLE NO 2
STANDARDS

VOKA1 AT NO 12 F(X)= .9213  T(P)/(E(Y)*C)= .99894-02  T(C)/I(P)= .89496-03  F(Y)*CON= .5571

STANDARDS COMPOUND STANDARD FOR ELEMENT 1

SIKA1 AT NO 12 F(X)= .6156  T(P)/(E(Y)*C)= .89202-02  T(C)/I(P)= .97003-03  F(Y)*CON= .3775

SOKA1 AT NO 14 F(X)= .8717  T(P)/(E(Y)*C)= .61757-02  T(C)/I(P)= .17078-02  F(Y)*CON= .5946

STANDARDS COMPOUND STANDARD FOR ELEMENT 2

FUKA1 AT NO 14 F(X)= .7578  T(P)/(E(Y)*C)= .60232-02  T(C)/I(P)= .18184-02  F(Y)*CON= .4051

FUKA1 AT NO 26 F(X)= .9756  T(P)/(E(Y)*C)= .19663-02  T(C)/I(P)= .24877-01  F(Y)*CON= .7754

POINT NO 1
K(1)= .1510
K(2)= .1184
K(3)= .1200

ELEMENT AT CONC WT CONC STD DEV F(X) I(P)/(E(Y)*C) I(C)/I(P) F(Y)*CON CHAR FLUOR F(X)CH4

NO 12 .3756 .2616 .0000 .4710 .00417-02 .1300-02 .3729 .76622-02 .5441
SI 14 .1811 .1010 .0000 .5657 .51591-02 .20591-02 .3149 .5441
FE 24 .0527 .1343 .0000 .9778 .17490-02 .42195-01 .5402
O 8 .5796 .4160 .0000

TOTAL = .0035

ITERATION NO 5

STOICHIOMETRY
8. References


APPENDIX 1

NBS Technical Note 521
PRESENT STATE OF THE CLASSICAL THEORY OF QUANTITATIVE ELECTRON PROBE MICROANALYSIS*

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Although the foundations for a procedure of data reduction in quantitative electron probe analysis have not been changed for several years, there has been progress in the choice of expressions, parameters, and constants. A brief account of recommended expressions and procedures is given. Reference is made to the Standard Reference Materials of Au-Ag and Au-Cu alloys issued for electron probe microanalysis. These are especially useful for investigating the application of correction procedures.

Key words: corrections; electron probe microanalysis; quantitative analysis; x-ray spectroscopy.

INTRODUCTION

In his doctoral thesis, published in 1951 [1], Castaing laid the groundwork for a theory of quantitative electron probe microanalysis. He pointed out that the intensity of characteristic primary radiation generated in multi-element specimens is approximately proportional to the mass fraction of the emitting element. He therefore proposed that the corrections which need to be applied to measured x-ray intensity ratios to obtain mass fractions ("concentrations") were as follows:

This paper is to appear in Mikrochim. Acta, in German, as part of the proceedings of a meeting on electron probe microanalysis and metallography, held in Vienna, (Technische Hochschule, Wien), October 22-25, 1969.
1. An absorption correction, which takes into account the absorption of x-rays emerging from the specimen, and

2. A fluorescence correction which cancels the effects of indirect x-ray generation.

Castaing also suggested that for accurate analysis the proportionality between concentration and intensity of emission may have to be considered an insufficient approximation. Hence, he proposed a form of atomic number correction to correlate more accurately the mass fraction with the measured intensity of x-ray emission.

This "classical" scheme of data reduction has essentially remained the commonly used approach to quantitative analysis. It has been described in many publications, including the National Bureau of Standards Special Publication 298 (1968) [2], which contains several references used in this paper. In the recent past there has been considerable discussion of the choice of parameters and constants to be employed within the framework of this procedure. The problem remains if, instead of the classical procedure, a Monte-Carlo method or a transport equation procedure is used to calculate the mass-fractions of the elements being measured.

It is the purpose of the present publication to give an account of the specific choices of parameters and constants which are available at present for the computation of corrections for quantitative electron probe microanalysis. For a general description of the correction procedures, as well as for a detailed discussion of the origin of these expressions, the reader is referred to the cited literature.
ATOMIC NUMBER CORRECTION

Thanks to the work of many investigators [e.g. 2-6] the processes resulting in primary x-ray emission are now quite well understood. The number of ionizations produced by a single electron coming to rest within the target can be written as follows:

\[ n_A = N_{Av} \cdot \rho \cdot \frac{C_A}{A} \int_{E_0}^{0} \frac{Q}{-dE/dx} \, dE \]  

(1)

For the ionization cross-section, \( Q \), and the stopping power, \( -dE/d(\rho x) \), we can substitute in the above equation the expressions proposed by Bethe et al. [7,8]:

\[ Q = b \cdot \pi e^4 \cdot z^4 \cdot \frac{\ln U}{U} \cdot E^{-2} \]  

(2)

\[ S = -\frac{1}{\rho} \cdot \frac{dE}{dx} = 2\pi e^4 \cdot N_{Av} \cdot \frac{Z}{A} \cdot \frac{1}{E} \cdot \ln \left( \frac{\alpha E}{J} \right) \]  

(3)

The values of some parameters of these equations are, however, poorly known. Hénoc has concluded from the study of experimental results on the ionization cross section that the value \( b = 0.76 \) can be considered valid for all levels of ionization [9]. The value of the coefficient \( \alpha \) in equation (3) was frequently considered to be equal to two. However, according to Nelms [10], for electrons the value \( \alpha = 1.166 \) should be used.

There is some controversy concerning the best expression for the mean ionization potential, \( J \). The value \((J = 11.5Z)\), used frequently in the past, is certainly inaccurate. We use at present an expression obtained by Berger and Seltzer [11], who averaged a large number of experimental observations by several authors:

\[ J = 9.76 \cdot Z + 58.5 \cdot Z^{-0.19} \]  

(4)

* A list of symbols used is appended.
Another expression for $J$ has been proposed by Duncumb et al. [12]:

$$J/Z = 14.0 \left[ 1 - \exp (-0.1 Z) \right] + 75.5/Z^{7.5} - Z/(100 + Z)$$  \hspace{1cm} (5)

This equation has been derived empirically to optimize the results of a large number of electron probe analyses of specimens of known composition. We withhold judgment on the best choice of expression for $J$, pending further investigations.

In order to obtain an algebraic expression for ionization within a multi-element target, we introduce the variables $M$ and $V$, defined by the following equations:

$$M = \sum_i C_i \frac{Z_i}{A_i} ; \quad V = \exp \left[ \frac{1}{M} \sum_i C_i \frac{Z_i}{A_i} \ln \left( \frac{\alpha E_i}{J_i} \right) \right]$$  \hspace{1cm} (6)

As shown by Springer [13], if one introduces equations (2), (3), and (6), the integration of equation (1) yields the expression

$$n_A = \frac{1}{2} \frac{C_A}{A} z_A b \left\{ U_o - 1 - \ln V \left[ EI(\ln U_o V) - EI(\ln V) \right] \right\}$$  \hspace{1cm} (7)

in which $EI$ is the exponential integral:

$$EI(x) = \text{const.} + \ln x + \sum_{s=1}^{\infty} \frac{x^s}{s \cdot s!}$$  \hspace{1cm} (8)

Expression (7) is used in an extensive program for data processing in quantitative electron probe microanalysis, called COR, recently developed by Hénoc and Heinrich at the National Bureau of Standards [14].

A further correction is necessary to take account of the effects of electron backscattering. A fraction of the impinging electrons is reemitted with energies sufficient to excite x-rays. This reduces the generated x-ray intensity by a fac-
tor R (backscatter effect), which decreases rapidly with increasing atomic number. The average number of ionizations per impinging electron is thus $n_A R$. We believe that the most reliable expression for the factor R is that proposed by Duncumb [15]:

$$R = 1.0000 +$$
$$+ (-0.581 \times 2.162 W - 5.137 W^2 + 9.213 W^3 - 8.619 W^4 + 2.962 W^5) \times 10^{-2} Z +$$
$$+ (-1.609 \times 8.298 W + 28.791 W^2 - 47.744 W^3 + 46.540 W^4 - 17.676 W^5) \times 10^{-4} Z^2 +$$
$$+ (5.400 \times 19.184 W - 75.733 W^2 + 120.050 W^3 - 110.700 W^4 + 41.792 W^5) \times 10^{-6} Z^3 +$$
$$+ (-5.725 \times 21.645 W + 88.128 W^2 - 136.060 W^3 + 117.750 W^4 - 42.445 W^5) \times 10^{-8} Z^4 +$$
$$+ (2.095 \times 8.947 W - 36.510 W^2 + 55.694 W^3 - 46.079 W^4 + 15.851 W^5) \times 10^{-10} Z^5$$

where $W = 1/U_0 = E_0/E_K$. This expression agrees well with the experimental measurements of the factor R by Dérian [16].

The number of photons of the x-ray line $n$, generated by ionization of the electron shell $m$, is obtained by multiplying the number of ionizations, $n_A R$, with the fluorescence yield, $\omega_m$, and with the ratio of the intensity of the line of interest to the intensity of all lines originating from this shell (weight of the line, $p_{mn}$):

$$I'_{\omega_p} = n_A \cdot R \cdot \omega_m \cdot p_{mn}$$

THE ATTENUATION OF PRIMARY RADIATION

The attenuation of primary radiation on emergence from the specimen can be calculated using an equation proposed by Philibert [17]

$$1/f(\chi) = (1 + \frac{\chi}{\sigma})(1 + \frac{h}{1+h} \cdot \frac{\chi}{\sigma}); \ h = 1.2 \frac{A}{Z^2}$$

The factor $f(\chi)$ is the ratio between attenuated and unattenuated primary radiation: $F(\chi) = I_p/I_p'$. Expressions for the coefficient $\sigma$, which depends on the electron energy, were pro-
posed by Duncumb and Shields [18] and by Heinrich [19]. We presently use the following equation:

\[ \sigma = \frac{4.5 \times 10^5}{E_0^{1.65} - E_k^{1.65}} \]  

(12)

We have not evaluated an alternative equation for the absorption correction, by Wittry and Andersen [20].

The attenuation of primary radiation is large when x-rays of low photon energy are measured. It is important to note, however, that the magnitude of this effect, and hence, the uncertainty of its computation, depends upon experimental conditions under our control. Primary absorption can be minimized by working at low electron energies and using high x-ray emergence angles; and these conditions are desirable when soft x-rays are measured. It should be added that further experiments on the depth distribution of primary x-rays should be encouraged. The uncertainties in the absorption correction have been analyzed by Yakowitz and Heinrich [21] who suggested that the experimental conditions should be adjusted, wherever possible, to maintain the value of \( f(\chi) \) above 0.8.

SECONDARY RADIATION EXCITED BY CHARACTERISTIC LINES

The effects of secondary radiation excited by characteristic lines are usually treated according to the equation proposed by Castaing [1]:

\[
\frac{r_f}{I_{PA}'} = \frac{C_B}{I_{PA}'} \cdot \frac{I_{PA}}{I_{PA}'} \cdot \frac{r_A - 1}{r_A} \cdot \frac{A}{B} \left[ \frac{\mu(A, BK\alpha)}{\omega_B} \cdot \frac{\mu(AB, BK\alpha)}{\omega_A} \right] \left[ \frac{f_n(1+u)}{u} + \frac{f_n(1+v)}{v} \right]
\]  

(13)

In this equation, \( r_f \) is the ratio of the attenuated fluorescent radiation to the attenuated primary radiation of the element which is being determined. \( I_{PA}' / I_{PB}' \) is the ratio of the gener-
ated (not attenuated) primary emissions of the exciting and the excited lines as obtained from pure elements. Castaing proposed to approximate this ratio by the ratio of the absorption edge wavelengths of these elements, while Reed [22] replaced it by the expression $[(U_B - 1)/(U_A - 1)]^{1.67}$ in which $U_A$ and $U_B$ are the corresponding overvoltage ratios.

This procedure is amenable to several improvements which were incorporated in the program COR. In this program, the ratio $I_B/I_A$ is fully calculated, using equation (10) for primary intensities, just as in the atomic number correction. This simplifies the calculation of fluorescence of K lines by L lines and vice versa, as well as the calculation of fluorescence of Kα lines by Kβ lines, which is performed separately. As pointed out by Criss [23], the exponential approximation to primary distribution in depth of x-ray emission, used by Castaing to calculate the term $v$ in equation (13), can be replaced by a more accurate model. We use in COR the model contained in Philibert's calculation for the function $f(x)$ [17]. With the computer facilities presently available to most analysts, this more rigorous approach is possible without an excessive increase in the cost of computation.

SECONDARY RADIATION EXCITED BY THE CONTINUUM

Hénoc has described a method for calculating the effects of secondary radiation excited by the continuum [24]. In order to perform the formal integration of the expressions contained in his procedure, he had to make the simplifying assumption that between absorption edges the mass attenuation coefficients vary with the cube of wavelength. However, the wavelength dependence of mass attenuation coefficients is always less than cubic [25]. This has been taken into account in the modification of Hénoc's original method incorporated
in the program COR. The formal integration is replaced by a numerical integration, using the parameters for attenuation coefficients published in reference [25].

The main practical difficulty in performing the correction for fluorescence excited by the continuum is that the position of the absorption edges of all elements contained in specimen and standard must be taken into account. Each wavelength range between adjacent absorption edges must be calculated separately. Therefore, the procedure is lengthy, and in machine computation it requires extensive data input. Errors in the input occur frequently and may escape detection, since it is difficult to acquire an intuitive feeling for the magnitude of this correction.

In the program COR the relations between lines and absorption edges are inspected by the computer which selects the wavelength ranges for the integration. These decisions are made and the computer completes the calculation without active intervention of the operator. In the same process, the computer also determines which operations must be performed for calculating secondary excitation by characteristic lines. This enormously simplifies the execution of the fluorescence corrections, and renders unnecessary further attempts to simplify them, as advocated by Springer [26].

**THE ITERATIVE PROCESS**

We will now discuss how the individual corrections are combined in calculating the composition of the specimen.

The usual form employs multiplicative correction factors:

\[ C^* = k \cdot k_z^* \cdot k_A^* \cdot k_F^* \]  (14)
This procedure is based on the concept that ideally the method should yield a linear correction curve. The multiplicative factors correct for deviations from the ideal model. However, the values of the correction factors depend on the composition of the specimen, which is unknown. The problem is traditionally resolved by using an estimate of composition to calculate the correction factors, and using the resulting mass fractions as a new estimate of composition and iterating until convergence of results is obtained.

As stated by Criss [23], the formulation of the correction by multiplicative factors unnecessarily complicates the structure of the correction equations, and obscures the underlying physical events. Moreover, the iteration frequently fails to converge, as observed by Reed [27]. For these reasons, the program COR uses a different iterative concept, first proposed by Criss and Birks [28], and somewhat modified by Hénoc and Heinrich.

Each iteration contains two steps. In the first step, we establish an estimate of the specimen composition and calculate the intensity ratios to be expected for each element, according to the theory. The intensity ratios are obtained by the simple relation

$$K = \frac{I^*}{I_{dp} + I_{dc} + \Sigma I^*_f} = \frac{I^*}{I_{dp} + I_{dc} + \Sigma I^*_f}$$

(15)

The correction procedures previously discussed are used to calculate the absolute intensities (in photons per electron) due to direct and indirect excitation. As a first estimate of the specimen composition we assume that the weight fractions of the elements are proportional to the experimentally obtained x-ray intensity ratios. This estimate, as well as the subsequent estimates is normalized so as to render the sum of mass fractions equal to unity. Thus, in each iteration, we calculate
the signal intensities to be expected from a theoretically possible composition.

Since equation (15) does not yield an explicit term for mass fractions, we must use another relation to obtain, in the second step of each iteration, a new estimate of composition. We use for this purpose a hyperbolic approximation to the analytical calibration curve for each element:

$$\frac{1-k}{k} = a \frac{1-C}{C}$$  \hspace{1cm} (16)

Ziebold and Ogilvie observed that the analytical curves in electron probe microanalysis are indeed approximately hyperbolic [29]. On the plot of intensity ratio versus mass fraction for each element, the hyperbola can be defined by three points (0,0), (1,1), and (C,k), where C and k are the estimate of mass fraction used in the iteration, and of the intensity ratio calculated for it. Our next estimate for the mass fraction, $C_m$, corresponding to the observed intensity ratio, $k_m$, can thus be calculated by the equation

$$C_m = \frac{k_m \cdot C(1-k)}{k_m(C-k) + k(1-C)}$$  \hspace{1cm} (17)

Contrary to the procedure suggested by Criss, we do not normalize the observed intensity ratios $k$ in equation (16), or the final results after convergence. Thus, if the presence of an element has been overlooked, or if there are experimental errors or failures of the correction procedures, this will become apparent since the calculated mass fractions fail to sum to unity.

This iteration procedure has been extensively tested. We have never observed failure to converge. In fact, the convergence is always rapid, as is to be expected in view of the good fit of the hyperbolic model observed by Ziebold and Ogilvie.
The program COR can also compute results of analysis with use of multi-element standards; furthermore it can determine one element by difference or several unmeasured elements on the basis of stoichiometric relations.

STANDARD REFERENCE MATERIALS

In spite of the progress made in recent years, there are still uncertainties in several aspects of the correction procedures. I believe that the availability of reliable standard reference materials will be instrumental in pointing out the areas in which further investigation is most needed. For this reason, the National Bureau of Standards has devoted considerable effort to preparing and characterizing materials specially selected for electron probe microanalysis [30]. Recently, NBS certified and issued an alloy of nominal composition 0.8 W, 0.2 Mo, a series of binary alloys in the Au-Ag system, in nominal steps of 0.2 (20 weight percent), and a similar series of alloys in the system Au-Cu. All these alloys were carefully analyzed chemically by several laboratories, and painstakingly investigated for homogeneity. They should be particularly useful in testing the atomic number correction. Extension of the studies of oxydric systems is presently in progress.
REFERENCES


### List of Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A, B)</td>
<td>atomic weights of elements (A, B)</td>
</tr>
<tr>
<td>(C)</td>
<td>mass fraction (&quot;concentration&quot;)</td>
</tr>
<tr>
<td>(E)</td>
<td>kinetic energy of the electron</td>
</tr>
<tr>
<td>(E_0)</td>
<td>initial kinetic energy of the electron, operating voltage</td>
</tr>
<tr>
<td>(E_k)</td>
<td>excitation potential of line (k)</td>
</tr>
<tr>
<td>(I)</td>
<td>attenuated (emergent) intensity of radiation</td>
</tr>
<tr>
<td>(I')</td>
<td>intensity of generated radiation, before attenuation</td>
</tr>
<tr>
<td>(J)</td>
<td>mean ionization potential</td>
</tr>
<tr>
<td>(M)</td>
<td>variable used for stopping power calculation (eq. 6-7)</td>
</tr>
<tr>
<td>(N_{Av})</td>
<td>Avogadro's number</td>
</tr>
<tr>
<td>(Q)</td>
<td>ionization cross-section</td>
</tr>
<tr>
<td>(R)</td>
<td>correction factor for electron backscattering</td>
</tr>
<tr>
<td>(S)</td>
<td>stopping power</td>
</tr>
<tr>
<td>(U)</td>
<td>(= \frac{E}{E_k})</td>
</tr>
<tr>
<td>(U_0)</td>
<td>(= \frac{E_0}{E_k})</td>
</tr>
<tr>
<td>(V)</td>
<td>variable used for stopping power calculation (eq. 6-7)</td>
</tr>
<tr>
<td>(W)</td>
<td>(= \frac{1}{U_0})</td>
</tr>
<tr>
<td>(Z)</td>
<td>atomic number</td>
</tr>
<tr>
<td>(a)</td>
<td>constant in the hyperbolic approximation</td>
</tr>
<tr>
<td>(b)</td>
<td>constant in the calculation of the ionization cross-section</td>
</tr>
<tr>
<td>(c)</td>
<td>constant in the calculation of (\sigma)</td>
</tr>
<tr>
<td>(e)</td>
<td>charge of electron</td>
</tr>
</tbody>
</table>
\( f(\chi) \) correction factor for absorption of primary radiation

\( h = 1.2(A/Z^2) \) in Philibert's equation. For multi-element targets, \( h = \sum c_i A_i / Z_i^2 \)

\( EI \) exponential integral

\( \ln \) natural logarithm

\( n_A \) number of ionizations produced by one electron which comes to rest within the specimen

\( p_{mn} \) relative frequency of the line \( n \), generated on ionization of the shell \( m \), with respect to generation of all lines originating from shell \( m \)

\( r \) absorption edge jump of the absorption coefficient

\( r_f \) intensity of emerging fluorescent radiation, relative to emerging primary radiation of the same line

\( s \) tally in the exponential integral

\( k \) relative intensity of emergent radiation

\( k_Z, k_A, k_F \) correction factors for atomic number, absorption, and fluorescence effects

\( u, v \) auxiliary variables for attenuation of fluorescent radiation

\( \alpha \) constant in Bethe's equation for energy loss of electrons

\( \theta \) emergence angle of measured x-rays

\( \mu \) x-ray mass attenuation coefficient

\( \mu(AB, AK\alpha) \) mass attenuation coefficient of specimen containing elements A and B, for K\(\alpha\) radiation of element A

\( \rho \) density of specimen

\( \sigma \) coefficient for electron energy effect in Philibert's equation

\( \chi = \mu \cosec \theta \)

\( \omega = \) fluorescence yield
Subscripts and superscripts:

A,B  elements A, B

i  tally in integration

1  electron shell 1

*  composition dependent
APPENDIX 2

Index of Terms and Symbols
Index of Terms and Symbols

This index is a list of variable names in the main program and in the subprograms, with an explanation of the use and meaning of the variable, and, where pertinent, with the equivalent symbol most commonly used in literature. Reference is made several times to the PTLOAD routine, which serves to enter data from a magnetic tape. This routine is specifically designed for the type of computer we use, and might have to be redesigned to enter data from magnetic tape in other installations.

In the manuscript, underlining has been used to distinguish the number 1 from the letter l. The following definitions, used in the explanatory notes, should be given here.

A run is a complete load of input cards. It usually consists of several cases. A case is a set of measurements of the same lines and elements, under identical conditions of excitation (operating voltage); in some of the measurements, one or more of the elements included in the case may be absent. Each case consists of a set of points. A point is a set of data corresponding to a single measurement, or to repeated measurements at the same location or at equivalent locations. For instance, in a run we may have one case consisting of measurements on stainless steel, and containing many points which may represent different specimens or points on specimens, and another case of brass analyses, again containing many points.

The summation signs in the explanations denote summation of the corresponding terms over all elements present in the specimen. Dummy variables have no effective functions, except to occupy spaces in memory arrays, so that other variables fall into the right places.
### Main Program

<table>
<thead>
<tr>
<th>Program Variable Name</th>
<th>Common Symbols</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(J)</td>
<td>A, B, etc.</td>
<td>Atomic weight of element, the atomic number of which is J</td>
</tr>
<tr>
<td>AI(JJA)</td>
<td>I(A)</td>
<td>Total emerging x-ray intensity from pure element A (See definition for JJA)</td>
</tr>
<tr>
<td>AIR(JJA)</td>
<td>$I_A^s/I(A)$</td>
<td>Ratio of emerging x-ray intensities from a compound standard, s, and from pure A</td>
</tr>
<tr>
<td>AIT</td>
<td>$I_A^x$</td>
<td>Total emerging x-ray intensity from the specimen for element A</td>
</tr>
<tr>
<td>AK(JJA)</td>
<td>$K_A$</td>
<td>Continuum efficiency constant (Kramer's constant)</td>
</tr>
<tr>
<td>AKEX(JJA)</td>
<td>$k_A = I_A^*/I(A)$</td>
<td>Ratio of experimental x-ray intensities emerging from specimen and pure A</td>
</tr>
<tr>
<td>ANK(J)</td>
<td>$n_K$</td>
<td>Exponent for calculating absorption coefficients for element J; in the equation: $\mu(J, \lambda) = C\lambda^n$ for $\lambda &lt; \lambda_K$ edge</td>
</tr>
<tr>
<td>ANKL(J)</td>
<td>$n_{KL}$</td>
<td>same, for $\lambda_K &lt; \lambda &lt; \lambda_L$</td>
</tr>
<tr>
<td>ATCO</td>
<td></td>
<td>Atomic fraction of each analyzed element</td>
</tr>
<tr>
<td>C(JJA),</td>
<td>$k_A, k_B, \ldots$</td>
<td>1. At start of the first iteration, and in the calculation of k-values: x-ray intensity ratio for each element.</td>
</tr>
<tr>
<td></td>
<td>$C_A, C_B, \ldots$</td>
<td>2. In all other instances: successive estimates of weight fraction of each element.</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>-----------------</td>
<td>-----------------------------------------------------------------------------</td>
<td></td>
</tr>
<tr>
<td>CC(JJ,JJA)</td>
<td>Absorption coefficient constant in $\mu(JJ,\lambda_{JJA})$ (definitions for JJ and JJA below).</td>
<td></td>
</tr>
<tr>
<td>CD(NP,JJA)</td>
<td>$k_j$ 1. Experimental x-ray intensity ratio for point NP, and line of JJA.</td>
<td></td>
</tr>
<tr>
<td>CI(J)</td>
<td>$C_j$ 2. (In the calculation of $k$-values) given concentration of element JJ.</td>
<td></td>
</tr>
</tbody>
</table>
| CL(L,K,J)       | $\lambda$ Wavelength of line:  
|                 | $L = $ line number  
|                 | $K = $ series number (edge)  
|                 | $J = $ atomic number |
| CO              | Weight fraction of an element determined by stoichiometry |
| CON(JJA)        | If the value of this variable is greater than zero for any element, the weight fraction of that element will be fixed at whatever is input on data cards. |
| COSEC(JJA)      | csc $\psi$ Cosecant of the x-ray emergence angle |
| CT(JJA)         | $C_A$ Approximation obtained as the result of each iteration (approximation number I+1 at the end of the Ith iteration) |
| ELNA(NZA)       | alphabetic variable Chemical symbol for an element of atomic number NZA (alphabetic) |
| EO              | $E_0$ Operating potential, in kV |

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<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EX(II,JJA)</td>
<td>Value of exponent for the absorption coefficient in ( \mu = C \lambda^n ), selected and stored by ( C0CA ). II = subinterval number, JJA = element label</td>
</tr>
<tr>
<td>EXPO(JJ,JJA)</td>
<td>Value of the exponent for the absorption coefficient at the wavelength ( \lambda ), corresponding to ( E_o [kV] ): ( (\lambda_o = \frac{12.398}{E_o}) )</td>
</tr>
<tr>
<td>FCASF(JJ)</td>
<td>Sum of emitted fluorescence intensities excited by characteristic lines, for element JJ</td>
</tr>
<tr>
<td>FCASFX</td>
<td>Sum of emitted characteristic fluorescence intensities, divided by the emitted primary intensity</td>
</tr>
<tr>
<td>FCF(JJ)</td>
<td>Emitted fluorescence intensity excited by the continuum, for element JJ</td>
</tr>
<tr>
<td>FCFX</td>
<td>Emitted continuum-fluorescence intensity divided by the emitted primary intensity</td>
</tr>
<tr>
<td>FCK12(J)</td>
<td>Coster-Kronig coefficients stored in the permanent data file for each element</td>
</tr>
<tr>
<td>FCK13(J)</td>
<td></td>
</tr>
<tr>
<td>FCK23(J)</td>
<td></td>
</tr>
<tr>
<td>FIRST</td>
<td>Logical variable used to label the first input card of a sample</td>
</tr>
<tr>
<td>FQC(JJ)</td>
<td>Absorption factor, ( f_c ), for fluorescence excited by the continuum</td>
</tr>
<tr>
<td>FQCA(JJ)</td>
<td>Absorption factor, ( f_f ), for the fluorescence x-ray intensity excited by characteristic lines</td>
</tr>
</tbody>
</table>
FQF(JJ) \quad f_p, f_p(x), f(x) \quad \text{Absorption factor for primary radiation, element JJ}

ICOF \quad \text{Switch to eliminate correction for continuum fluorescence}

III \quad \text{Constant needed for reading magnetic tape input via PTLOAD (not operative unless PTLOAD is used)}

IMA(JJA) \quad \text{Number of sublimits needed in the calculation of fluorescence excited by the continuum}

J \quad Z \quad \text{Subscript for atomic number}

JJ \quad \text{Subscript for order in which the element appears in the input data (arbitrary) = "element label"}

JJA \quad \text{Label JJ of the element being measured}

JJA_1, JJA_2 \quad \text{Element labels of unanalyzed elements}

JJAM \quad \text{Number of analyzed elements}

JJAS \quad \text{JJJ + 1}

JJJ(I,JJA) \quad \text{Label of the element which emits the line of wavelength WAVE(I,JJA)}

JJM \quad \text{Number of elements in a case}

JJMX \quad \text{Either JJAM or JJM, depending on the variant of the program}

JST \quad \text{Number of elements contained in a compound standard}

K \quad \text{Subscript: level number (edge)}
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>KA(JJA)</td>
<td>Number of the level of the analyzed element which emits the measured line</td>
</tr>
<tr>
<td>KAA</td>
<td></td>
</tr>
<tr>
<td>KB(I,JJA)</td>
<td>Number of the level emitting the line WAVE(I,JJA)</td>
</tr>
<tr>
<td>KK</td>
<td>Diverse switches</td>
</tr>
<tr>
<td>KM(J)</td>
<td>Number of absorption edges listed in the permanent data file, for element J</td>
</tr>
<tr>
<td>KMJ</td>
<td></td>
</tr>
<tr>
<td>KSTOP</td>
<td>Switch for termination of program</td>
</tr>
<tr>
<td>L</td>
<td>Subscript for CL(L,K,J). Position in the sequence in which the lines are</td>
</tr>
<tr>
<td></td>
<td>filed in the permanent data file. This sequence restarts after each edge.</td>
</tr>
<tr>
<td>LA(JJA)</td>
<td>Subscript: Position of measured line in permanent data file.</td>
</tr>
<tr>
<td>LI(KAA,LAA)</td>
<td>Name of analyzed line (KA1_, MB1_, ..., etc.)</td>
</tr>
<tr>
<td>LM(K,J)</td>
<td>Number of lines listed in the series K, of the element of atomic number J</td>
</tr>
<tr>
<td>LMKJ</td>
<td>(K=level number of the edge).</td>
</tr>
<tr>
<td>LOUT</td>
<td>Switch for output 2.</td>
</tr>
<tr>
<td>MESS(JJ,JJA)</td>
<td>Switch for writing error message</td>
</tr>
<tr>
<td>MF(JJA)</td>
<td>Number of characteristic lines which excite fluorescent emission</td>
</tr>
<tr>
<td>NCO(JJA)</td>
<td>Switch for error termination due to insufficient data</td>
</tr>
</tbody>
</table>
Switch for input method
Case number
Number of cases in a run
Number of elements listed in table
Number of additional elements in a compound standard (not including the analyzed element)
Number of iteration
Running number of element for reading permanent data file.
Index: data point number in any case
Total number of data points minus 1
Total number of data points
Switch determining the variant of the program to be used
Switch set for terminating iterations
Magnetic tape assignment (for PTLOAD only)
Valence of element number JJ
Subscripts for stoichiometry printout
Atomic number of element JJ
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>NZA</td>
<td>Atomic number for a particular element</td>
</tr>
<tr>
<td>NZA1</td>
<td></td>
</tr>
<tr>
<td>NZEX</td>
<td></td>
</tr>
<tr>
<td>NZO</td>
<td></td>
</tr>
<tr>
<td>OME(K,J)</td>
<td>$\omega_q(J)$</td>
</tr>
<tr>
<td>OMEG(I,JJA)</td>
<td>$\omega_{\text{eff}}$</td>
</tr>
<tr>
<td>R(K,J)</td>
<td>$r_q$</td>
</tr>
<tr>
<td>RPF(JJ)</td>
<td>$I_p$</td>
</tr>
<tr>
<td>RPFX</td>
<td></td>
</tr>
<tr>
<td>RR(I,JJA)</td>
<td>$r_i$</td>
</tr>
<tr>
<td>RRR(I,JJA)</td>
<td>$(r_i-1)/r_j$</td>
</tr>
<tr>
<td>SA1</td>
<td></td>
</tr>
<tr>
<td>SACO</td>
<td>$\Sigma(C_i/A_i)$</td>
</tr>
<tr>
<td>SC</td>
<td>$\Sigma C_i$</td>
</tr>
<tr>
<td>SD(NP,JJ)</td>
<td>$\sigma_k$</td>
</tr>
</tbody>
</table>

*Fluorescence yield for level number K of element of atomic number J*  
*Effective yield for ionization produced by photons (corrected for Coster-Kronig effects)*  
*Jump ratio at edge number K of element of atomic number J*  
*Emitted primary intensity of element number JJ*  
*Generated primary intensity of an element*  
*Absorption jump ratio associated with line of wavelength WAVE(I,JJA)*  
*Jump-efficiency ratio for element JJA*  
*Auxiliary variable in calculation of atomic concentration*  
*Sum of the weight fractions divided by their respective atomic weights*  
*Summation of the weight fractions*  
*Relative standard deviation of the k-value of element JJ for point number NP (used only when raw data are input)*
STOIC
Weight fraction of oxide in stoichiometric compound

SWITCH
Switch used in composing the output

WA(JJA) \( \lambda_o = \frac{12.398}{E_o} \)
Minimum wavelength of continuum emission, related to the incident electron energy \( E_o \) for element JJA

WAV(K,J) \( \lambda_q \)
Edge wavelength of the absorption edge of level number K, of the element of atomic number J

WAVE(I,JJA) \( \lambda_{q,m} \)
Wavelength of a characteristic line of element JJA

ZL(L,K,J) \( p_{q,m} \)
Weight of line with respect to the sum of line intensities in its series: \( L = \) line number, \( K = \) series or level number, \( J = \) atomic number

All variables named:

\( D_1, D_2, \ldots \) or \( N_1, N_2, \ldots \) are dummy variables used only to keep variables in COMMON in order.
### Additional Variables in AINP

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASUM</td>
<td>Average value of a set of peak- or background-intensity measurements</td>
</tr>
<tr>
<td>C(I,J,II)</td>
<td>$k_j$</td>
</tr>
<tr>
<td>COUNT</td>
<td>Count-rate, in cts/sec, for dead-time correction</td>
</tr>
<tr>
<td>CSTD(I,J)</td>
<td>Intensity of standard, corrected for dead-time</td>
</tr>
<tr>
<td>DEADT(---)</td>
<td>Function used to make dead-time correction</td>
</tr>
<tr>
<td>FSD(J,I)</td>
<td>Double-precision standard relative deviation of counts collected for each element in each point</td>
</tr>
<tr>
<td>I</td>
<td>Index</td>
</tr>
<tr>
<td>IC</td>
<td>$IC = ICON(I,J)$</td>
</tr>
<tr>
<td>ICON(I,J)</td>
<td>Number of times standards or backgrounds are read</td>
</tr>
<tr>
<td>I,IIC</td>
<td>Index</td>
</tr>
<tr>
<td>IIMAX</td>
<td>$IIMAX = JJAM$ (number of elements analyzed)</td>
</tr>
<tr>
<td>IJ</td>
<td>$IJ = NPM$ (total number of data points)</td>
</tr>
<tr>
<td>IK</td>
<td>$IK = 6-I$ (tally for separating of codes for scalers)</td>
</tr>
<tr>
<td>IND</td>
<td>Variable for dead-time determination</td>
</tr>
<tr>
<td>INDEX</td>
<td>An index for setting up a table of all the input data</td>
</tr>
<tr>
<td>ITEN</td>
<td>$ITEN = 10^{IK}$ auxiliary variable for scaler code separation</td>
</tr>
</tbody>
</table>
KK(J)  Counter for number of determinations in each point
M  \( M + NC \times ND \)
MCO(I)  Variable used in separating data code
NAV  Output code: if 0, print: average of measurement for each point
if 1, handle all data individually as separate points
NC  Number of scalers used in a measurement
NC1  \( NC_1 = NC - 1 \)
NCODE(NROW,I)  \( NCODE(NROW,I) = \frac{MCO(I)}{ITEM} \)
NCOL  Index (number of columns)
ND  Total number of lines or cards in input (including standards and background measurement)
NIND  Indicator which selects the proper dead-time for each spectrometer
NM  Position of data coder
(NM = NC-- (coding must be in the last position))
NR  \( NR = NSTD(IIC,1, I,J) \)
NROW  Index (number of lines)
NS  Number of digits per scaler (NS=6)
NSTD(...)  Various sub-tables of NTABL (NROW,I)
NTABL(NROW,I)  Complete table of all input data
If NTC=0, data are on magnetic tape
If NTC=1, data are on cards
If NTRA=0, calculate using total counts
If NTRA=1, calculate using counts/sec
List of numbers returned by magnetic-tape reading subroutine PTLOAD
Peak minus background for standards
Peak intensity of specimen
Sum of the standard intensities (peak or background)
Sum of peak intensities on each point of the specimen
Average peak intensity on each point of the specimen
Conversion of STSD from double precision to single
Sum of the squares of all peak and background measurements for each standard (double precision)
Relative double precision standard deviation for signals from each standard and background
Sum of all peak and background measurements for each standard (double precision)

\[
SUMS(I,J) = \frac{[SUM(I,J)]^2}{ICON(I,J)} \quad \text{(double precision)}
\]
Time in seconds
Summation of times in each point
### Additional Variables in COCA

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_{12}$</td>
<td>$f_{12}$ Coster-Kronig coefficients</td>
</tr>
<tr>
<td>$F_{13}$</td>
<td>$f_{13}$</td>
</tr>
<tr>
<td>$F_{23}$</td>
<td>$f_{23}$</td>
</tr>
<tr>
<td>$I$</td>
<td>Subscript: index of sub-limits of the wavelength ranges</td>
</tr>
<tr>
<td>$I_2$</td>
<td>Number of absorption edges of one element between $\lambda_0$ and $\lambda_m$</td>
</tr>
<tr>
<td>$I_3$</td>
<td>Number of the exciting line (char. fluor.)</td>
</tr>
<tr>
<td>$I_{3M}$</td>
<td>Total number of exciting lines (char. fluor.)</td>
</tr>
<tr>
<td>$II$</td>
<td>Subscript: index of sub-limits</td>
</tr>
<tr>
<td>$IL$</td>
<td>$IM-I+1$ Variable value for $I$ in loop</td>
</tr>
<tr>
<td>$IM$</td>
<td>$IM_1 = IM-1$</td>
</tr>
<tr>
<td>$JM$</td>
<td>For pure element standard: $JM = JJA$ For compound standard: $JM = JST$ For specimen: $JM = JJM$</td>
</tr>
<tr>
<td>$JO$</td>
<td>For all standards: $JO = JJA$ For all specimens: $JO = 1$</td>
</tr>
</tbody>
</table>
Auxiliary variables related to shells and subshells:

<table>
<thead>
<tr>
<th>K</th>
<th>KR1</th>
<th>KR2</th>
<th>K1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>9</td>
<td>5</td>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>7</td>
<td>1</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>7</td>
<td>1</td>
</tr>
<tr>
<td>12</td>
<td>7</td>
<td>8</td>
<td>5</td>
</tr>
</tbody>
</table>

Variable M4 = IM1

Jump ratio: NNR = R(K,J)

Temporary storage

λo wavelength: WAA = WA(JJA)
Additional Variables in CALI

FCAS \( \Sigma I^*_f \) Total fluorescence intensity excited by characteristic lines (emitted)

FCASO \( \Sigma I'_f \) Total fluorescence intensity excited by characteristic lines (generated)

FQ \( f_p, f(x) \) Absorption factor for primary emission

FQCA \( f_f, f(x)_{\text{char}} \) FQCA \( = FQCA(JJ) \)

FQCF(JJA) \( f_c f(x)_c \) FQCF(JJA) \( \equiv FQC(JJ) \)

IMAM \( \) IMAM \( = \text{IMA}({JJA}) \)

IO \( \) IO \( = \text{IMA}({JJA})+1 \)

RP \( I_p \) Emerging primary intensity = RPF(JJ)

RPO \( I'_p \) Generated primary intensity
### Additional Variables for FCA

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_A^*$</td>
<td>$\chi_A^* = \sum B \mu(B, A \text{qm}) X$</td>
</tr>
<tr>
<td>$\chi_B^*$</td>
<td>$\chi_B^* = \sum B \mu(B, A \text{qm}) X$</td>
</tr>
<tr>
<td>$\mu_B^A$</td>
<td>$\mu_B^A = C_i^A \left(\lambda_B^i\right)^n_i$</td>
</tr>
<tr>
<td>$a_i, b_i$</td>
<td>Coefficients of expansion of the depth-distribution function $\phi(\rho z)$ (according to Criss [5]): $\phi(\rho z) = \sum a_i \exp \left[-b_i \rho z\right]$</td>
</tr>
<tr>
<td>$I_f$</td>
<td>Fluorescence intensity excited by a characteristic line (emitted)</td>
</tr>
<tr>
<td>$I_f'$</td>
<td>Fluorescence intensity excited by a characteristic line (generated)</td>
</tr>
<tr>
<td>$f_f$</td>
<td>Absorption factor in fluorescence intensity excited by a characteristic line</td>
</tr>
<tr>
<td>$h$</td>
<td>$h$ from Philibert's absorption correction equation</td>
</tr>
<tr>
<td>$J$</td>
<td>Number of the exciting element</td>
</tr>
<tr>
<td>$KBB$</td>
<td>$KBB = KB(I, JJA)$</td>
</tr>
<tr>
<td>$LBB$</td>
<td>$LBB = LB(I, JJA)$</td>
</tr>
<tr>
<td>$NZB$</td>
<td>Atomic number of exciting element</td>
</tr>
<tr>
<td>$RJ$</td>
<td>Conversion of $J$ from integer to real mode</td>
</tr>
</tbody>
</table>
Step in calculation of fluorescence intensity excited by characteristic lines (emitted)

S2
Step in calculation of fluorescence intensity excited by characteristic lines (emitted)

S0
Step in calculation of fluorescence intensity excited by characteristic lines (generated)
Additional Variables in CO

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC(CL,J)</td>
<td>Mass absorption coefficient of element J, for the wavelength: γ = CL (function)</td>
</tr>
<tr>
<td>ACS</td>
<td>$X^*_A = \sum C_B \mu(B,A qm) X \cos \psi$</td>
</tr>
<tr>
<td>ALK</td>
<td>Conversion of LK from integer to real mode</td>
</tr>
<tr>
<td>ANIN</td>
<td>Conversion of NIN from integer to real mode</td>
</tr>
<tr>
<td>ANZ</td>
<td>Conversion of NZ from integer to real mode</td>
</tr>
<tr>
<td>BK1, BK2</td>
<td>Sublimits used in the computation of the definite integral over wavelength</td>
</tr>
<tr>
<td>BN, BN1, BO</td>
<td></td>
</tr>
<tr>
<td>CCO(J)</td>
<td>Value of $C_i$ (constant for calculation of $\mu$) for element J, as a function of wavelength</td>
</tr>
<tr>
<td>EABI</td>
<td>Auxiliary variable in the calculation of fluorescence excited by the continuum</td>
</tr>
<tr>
<td>EXO(J)</td>
<td>Value of exponent $n_i$ for element J</td>
</tr>
<tr>
<td>F(X,J0,JM,JJA)</td>
<td>Auxiliary function for numerical integration (emitted)</td>
</tr>
<tr>
<td>FC</td>
<td>Fluorescence intensity excited by the continuum (emitted)</td>
</tr>
<tr>
<td>FCO</td>
<td>Fluorescence intensity excited by the continuum (generated)</td>
</tr>
<tr>
<td>FI</td>
<td>Step in calculation of FC</td>
</tr>
</tbody>
</table>
Step in calculation of FCO

Auxiliary function for numerical integration, case without absorption

Wavelength increment for integration

IM1 = IMA(JJA)

Index

Limit of LK

Number of intervals used in the integration

NIN = 2*NIN2

Effective yield in a given interval of wavelength

Remainder after wavelength interval is divided

RRRI = RRR(I,JJA)

Step in calculation of fluorescence excited by the continuum (emitted)

Step in calculation of fluorescence excited by the continuum (generated)

Efficiency constant for continuum production
Additional Variables in RB

R1 to R5

W

1/U₀

W2 to W5

(1/U₀)² to (1/U₀)⁵

Z₁ to Z₅

Z₁ = 1x10⁻²Z; ... Z₅ = 1x10⁻¹₀Z₅

Auxiliary variables in calculation of backscatter

Reciprocal of overvoltage

Powers of W

Additional Variables in FQI

H

h

h from Philibert's equation

SIG

σ

σ = 4.5x10⁻⁵/(E₀₁·65-E₁·65)

Additional Variables in EI

AN

Conversion of N from integer to real mode

N

Index

TN

Step in calculation of exponential integral

X

Function to be integrated (ALUOW or ALW)
Additional Variables in FT

DACS

Dummy variable in COMMON

Additional Variables in AC

AN

Conversion of N from integer to real mode

Additional Variables in PRA

ALUOW

\[ \ln(U_0 V) \]

\[ \ln(U_0 V) = \ln(U_0) + \ln(V) \]

ALW

\[ \ln(V) \]

\[ \ln(V) = \sum_{A,B} C_i \frac{Z_i}{A_A} \ln X \]

\[ X \left( \frac{1.166E}{J_i} \right) / \sum_{A,B} C_i \frac{Z_i}{A_A} \]

AM

\[ M \]

\[ M = \sum_{A,B} C_i \frac{Z_i}{A_A} \]

AMLW

\[ M \ln(V) \]

\[ M \ln(V) = \sum_{A,B} C_i \frac{Z_i}{A_A} \ln X \]

\[ X \left( \frac{1.166E}{J_i} \right) \]

AW

\[ V \]

\[ V = \exp [ALW] \]

CX

\[ C_A \]

Concentration of analyzed element

EI

\[ \text{ei}(x) \]

Function: \[ \text{ei}(x) = \int_{-\infty}^{x} e^{\frac{V}{V}} dV \]

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EM
JX
KX
KXX
LX
OMED
RB
RBA
RZ
UO
Z
ZJ
ZNL

$E_1$
$Z_A$
Subscript: level number (edge) = K
KX must be greater than 4:

\[
\begin{array}{ccc}
KX & KXX \\
5 & 1 \\
6 & 1 \\
7 & 2 \\
8 & 2 \\
9 & 3 \\
\end{array}
\]

Subscript: line number = L
Effective fluorescence yield for ionization produced by electrons
Backscatter factor
Conversion of NZ from integer to real
Overvoltage
Atomic number
Mean excitation potential
Number of electrons in a shell
Additional Variables in F

\[ \mu_A = C_i(\lambda Z)^n_i \]

Mass absorption coefficient, pure element:

\[ \mu^*(\lambda) = \sum_{A,B} A[B][C_i(\lambda)^n_i] \]

Mass absorption coefficient, specimen

Whichever sublimit is used in the calling routine (BK1, BK2, BN, BN1, or BO)

\[ X \]

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APPENDIX 3

Permanent Data File
Permanent Data File

Types of cards for data input to the permanent data table

<table>
<thead>
<tr>
<th>Card No.</th>
<th>When Used</th>
<th>Cols.</th>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>once at beginning of table</td>
<td>1-3*</td>
<td>(I3)</td>
<td>Number of elements in permanent data table</td>
</tr>
<tr>
<td>2</td>
<td>first card for each element</td>
<td>1-2*</td>
<td>(I2)</td>
<td>atomic number</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3-4*</td>
<td>(I2)</td>
<td>number of absorption edges listed in table</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5-10</td>
<td>(F6.3)</td>
<td>atomic weight</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3F6.4)</td>
<td>Coster-Kronig coefficients</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$f_{12}$, $f_{23}$, $f_{13}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>29-34</td>
<td>(F6.2)</td>
<td>absorption constant $C_i$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2 fields of 4</td>
<td>(2F4.2)</td>
<td>absorption exponents $n_K$, $n_{KL}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(35-42)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>card for each edge</td>
<td>1-7</td>
<td>(F7.5)</td>
<td>wavelength at absorption edge</td>
</tr>
<tr>
<td></td>
<td></td>
<td>8-13</td>
<td>(F6.4)</td>
<td>jump for the edge</td>
</tr>
<tr>
<td></td>
<td></td>
<td>14-19</td>
<td>(F6.5)</td>
<td>fluorescent yield $\omega$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20</td>
<td>(I1)</td>
<td>number of lines listed for the edge</td>
</tr>
<tr>
<td>4</td>
<td>card for each line</td>
<td>1-7</td>
<td>(F7.5)</td>
<td>wavelength of line</td>
</tr>
<tr>
<td></td>
<td></td>
<td>8-13</td>
<td>(F6.4)</td>
<td>weight of the line with respect to the sum of line intensities in its series</td>
</tr>
</tbody>
</table>

*Number must be right justified in the field.
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<table>
<thead>
<tr>
<th>1</th>
<th>1007</th>
</tr>
</thead>
<tbody>
<tr>
<td>120.</td>
<td>6939</td>
</tr>
<tr>
<td>111.</td>
<td>9012</td>
</tr>
<tr>
<td>676</td>
<td>1081</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6</th>
<th>12011</th>
</tr>
</thead>
<tbody>
<tr>
<td>4368</td>
<td>2622</td>
</tr>
<tr>
<td>447</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>7</th>
<th>14007</th>
</tr>
</thead>
<tbody>
<tr>
<td>3099</td>
<td>2576</td>
</tr>
<tr>
<td>316</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
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### A Rigorous Correction Procedure for Quantitative Electron Probe Microanalysis (COR 2)

#### 16. ABSTRACT

This publication describes a rigorous data reduction procedure for quantitative electron probe microanalysis, which avoids simplifications present in conventional schemes. In addition, the program contains a correction for fluorescence due to the continuum, and separate computation of the fluorescent effects of each exciting primary x-ray line. Constants characteristic of elements are stored in a permanent data file, and the constants and parameters needed for the calculation of mass absorption coefficients are contained in a sub-program. These provisions and decision-making sections in the development of the fluorescence corrections reduce the required input considerably.

#### 17. KEY WORDS

Continuum fluorescence; data reduction; electron probe microanalysis; fluorescence correction; quantitative analysis.

#### 18. AVAILABILITY STATEMENT

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